Semiclassical analysis coherent states ergodic theory and a flavor of quantum chaos

Monique Combescure

Semiclassical Analysis, Coherent States, Ergodic Theory and a flavor of Quantum Chaos

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Monique Combescure

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Analyse semi-classique, états cohérents, théorie ergodique et un soupçon de "chaos quantique"

À destination d'un auditoire d'étudiants de 3ème cycle ayant une formation en physique théorique ou en physique-mathématique, ce cours a pour objet d'introduire d'une manière simple les outils et résultats principaux de "l'analyse semi-classique", comme un pont, lorsque la constante de Planck peut être considérée comme petite, entre les formalismes de la Mécanique Classique et de la Mécanique Quantique.

En particulier on donnera une approche aussi "pédestre" que possible de l'analyse dite microlocale (dans l'espace de phase), des transformations symplectiques et de leurs équivalents quantiques du groupe "métaplectique", de la propagation des états cohérents (et états "comprimés"), du théorème d'Égorov pour la propagation d'observables, de la quantification de Weyl et de la Transformation de Wigner.

Dans un deuxième temps, après un rappel rapide des bases de la théorie ergodique, on présentera des résultats importants dans le domaine dit du "chaos quantique", notamment le Théorème de Schnirelman et des formules de trace type "Gutzwiller" (ou "Balian-Bloch").

RÉSUMÉ

Chapitre 1

Quantum, Classical and Semiclassical Observables

1.1 Hamiltonian Classical Mechanics

1.1.1 The Classical Hamiltonian Flow

$X := \mathbb{R}^n$ is the configuration space (n degrees of freedom)
$Z := X \times X^*$ is the phase space
$q \in \mathbb{R}^n$ is a generic point in configuration space
$p \in \mathbb{R}^n$ is a generic momentum
$z := (q, p)$ is a generic phase space point
We define the **symplectic form**

Definition 1.1.1 *Given two phase-space points $z = (q, p) \quad , z' = (q', p')$, their symplectic product is given by :*

$$\sigma(z, z') = q.p' - p.q' = z.Jz' \tag{1.1}$$

where the dot . denotes either scalar product in $\mathbb{R}^n$ or in $\mathbb{R}^{2n}$, and J is the $2n \times 2n$ **symplectic matrix** *:*

$$J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \tag{1.2}$$

and $\mathbb{1}$ is the unit $n \times n$ matrix.

Classical Hamiltonian H :

$H: \quad Z \mapsto \mathbb{R}$ is regular enough. Basic example :

$$H(q,p) = \frac{p^2}{2m} + V(q)$$

of the usual kinetic plus potential energy function, ($m > 0$ being the mass of a particle).

The Hamilton equations read :

$$\dot{q} = \nabla_p H \qquad \dot{p} = -\nabla_q H \tag{1.3}$$

and generate the "classical flow"

$$\phi_H^t : \qquad Z \mapsto Z$$

(note that the overdot denotes differentiation with respect to time t).

$$\phi_H^t(q,p) = (q(t), p(t))$$

with initial data $q(0) = q, \qquad p(0) = p$, that is $\phi_H^0 = \mathbb{1}$ (the identity map in Z).

Note that : Cauchy-Lipschitz theorem $\Rightarrow$ Local existence

More assumptions on $H \qquad \Rightarrow$ Global existence of the flow.

Proposition 1.1.2 *The classical Hamiltonian flow obeys the following invariance properties :*

(i) σ is invariant under ϕ_H^t :

$$\sigma(q(t), p(t)) = \sigma(q,p)$$

(ii) ϕ_H^t preserves volumes of phase-space :

$$|\phi_H^t(M)| = |M|$$

where $|M|$ denotes the Lebesgue measure of a set $M \subset Z$.

(iii) Energy conservation : the energy surface :

$$\Sigma_E := H^{-1}(E) = \{z \in Z : \quad H(z) = E\}$$

is invariant under ϕ_H^t

$$z \in \Sigma_E \Rightarrow \phi_H^t(z) \in \Sigma_E$$

Definition 1.1.3 *E is a critical energy for H if $\nabla_z H = 0$ on Σ_E.*

Definition 1.1.4 *If E is not a critical value for H, we can define the* **Liouville measure** *on Σ_E :*

$$dL_E := \frac{d\Sigma_E}{|\nabla_z H|} \tag{1.4}$$

where $d\Sigma_E$ is the Euclidean measure on Σ_E.

Lemma 1.1.5 *Let E be a non-critical energy point for H. The Liouville measure dL_E is invariant under ϕ_H^t.*

Proof : let f be a regular function $Z \mapsto \mathbb{R}$, with compact support, such that its support doesn't contain any critical value. We have :

$$\int_Z f(z)dz = \int_{\mathbb{R}} dE \left(\int_{d\Sigma_E} dL_E(z) f(z) \right)$$

Then $\forall E_0$ we have :

$$\frac{d}{dE} \int_{E_0 \leq H(z) \leq E} f(z)dz = \frac{d}{dE} \int_{E_0}^{E} \left(\int_{\Sigma_E} dL_E(z) f(z) \right) = \int_{\Sigma_E} dL_E(z) f(z)$$

Since ϕ_H^t preserves volumes in Z, the measure dL_E is also invariant under ϕ_H^t.

Definition 1.1.6 *A is called a* **classical observable** *: if $A : \quad Z \mapsto \mathbb{R}$ is a sufficiently smooth function (say $A \in \mathcal{S}(\mathbb{R}^{2n})$)*

Definition 1.1.7 *The* **Poisson bracket** *of two classical observables A , B is defined as follows :*

$$\{A, B\} := \nabla A \ . \ J \nabla B \tag{1.5}$$

Lemma 1.1.8 *Let A be a classical observable. We have :*

$$\frac{d}{dt} A(z_t) = \frac{d}{dt} (A \circ \phi_H^t)(z) = \{H, A\} \circ \phi_H^t(z) \tag{1.6}$$

Proposition 1.1.9 *The Hamiltonian flow obeys the following properties :*
(i) Equ (1.3) is equivalent to (1.6)
(ii) The Poisson bracket is invariant under ϕ_H^t
(iii) A classical observable A is constant along a classical trajectory generated by ϕ_H^t iff $\{A \ , \ H\}$ vanishes along this trajectory.

1.1.2 The symplectic structure of the Phase Space

Let M be a real $2n \times 2n$ matrix, and denote by $\tilde{M}$ the transpose of M.

Definition 1.1.10 *M is said to be a* **symplectic matrix** *if* $\sigma(Mz, Mz') = \sigma(z, z') \qquad \forall z, z' \in Z$ *or equivalently*

$$\tilde{M} J M = J \tag{1.7}$$

Note that J is itself symplectic, since $\tilde{J} = -\mathbb{1}, \qquad J^2 = -\mathbb{1}$

Exercise Using the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

construct for $n = 1$ as many symplectic matrices as possible, and give a geometric interpretation.

Proposition 1.1.11 *The set Sp(n) of all symplectic matrices is a multiplicative group. Furthermore, we have :*
(i) $\det M = 1$
(ii) the characteristic polynomial of M is recurrent, namely

$$P(\lambda) = \lambda^{2n} P(1/\lambda)$$

where $P(\lambda) := \det(M - \lambda\mathbb{1})$.

Corollary 1.1.12 *Let $M \in Sp(n)$. It λ is eigenvalue of M, then :*
(i) $1/\lambda$ is also eigenvalue of M
(ii) $\bar{\lambda}$ is also eigenvalue of M

Exercise It is often useful to decompose M into 4 blocks of $n \times n$ matrices :

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

What are the properties that A, B, C, D must satisfy in order that $M \in Sp(n)$?

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1.2 Quantum dynamics

1.2.1 Known preliminaries

The traditional Hamiltonian for the Schrödinger equation is :

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(x) \tag{1.8}$$

Where Δ is the laplacian in $\mathbb{R}^n$, and $V: \quad \mathbb{R}^n \mapsto \mathbb{R}$.
We shall put a hat on letters to mean that they are operators in the space $\mathcal{H} := L^2(\mathbb{R}^n)$ of quantum states.

Mathematical digression : What is an **Operator** in a Hilbert space $\mathcal{H}$? It is a linear application $\mathcal{H} \mapsto \mathcal{H}$. In general, since $\mathcal{H}$ is of infinite dimension, the operators are **unbounded** For example if $n = 1$ the operator $\hat{X}$: $\varphi(x) \mapsto x\varphi(x)$ is unbounded. Namely in order that $x\varphi \in \mathcal{H}$, it is necessary that φ has enough decrease at infinity. Similarly $\hat{P}: \quad \varphi(x) \mapsto -i\hbar\frac{d}{dx}\varphi(x)$ (where the last expression is defined a priori in a distributional sense since $L^2 \subset L^1_{loc}$) is bounded provided the Fourier Transform of φ has enough decrease at infinity. If an operator $\hat{A}$ is unbounded, there nevertheless exists a subspace of $\mathcal{H}$ called *domain* of $\hat{A}$ and denoted $\mathcal{D}(\hat{A})$ such that

$$\varphi \in \mathcal{D}(\hat{A}) \Rightarrow \hat{A}\varphi \in \mathcal{H}$$

In general we are interested only in operators whose domains are dense in $\mathcal{H}$.

For **unbounded** operators, the property of being *selfadjoint* is not equivalent to that of being *hermitian* :

hermitian : $\langle \hat{A}\varphi\ , \psi\rangle = \langle \varphi\ ,\ \hat{A}\psi\rangle \quad \forall \varphi, \psi \in \mathcal{D}(\hat{A})$
selfadjoint We must have in addition that $\mathcal{D}(\hat{A}^*) = \mathcal{D}(\hat{A})$ where $\varphi \in \mathcal{D}(\hat{A}^*)$ *if* $\exists g \in \mathcal{H}$ such that $\langle \varphi, \hat{A}\psi\rangle = \langle g, \psi\rangle \qquad \forall \psi \in \mathcal{D}(\hat{A})$. g is unique and denoted $g := \hat{A}^*\varphi$.
Above and in all that follows we use the following definition :

Definition 1.2.1 *By $\langle ., \ .\rangle$ we denote the usual scalar product in $L^2(\mathbb{R}^n)$:*

$$\langle \varphi, \psi\rangle := \int_{\mathbb{R}^n} dx \bar{\varphi}(x)\psi(x)$$

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Under rather general assumptions on the potential V :
one can show that $\hat{H} = -\frac{\hbar^2}{2m}\Delta = V$ is essentially selfadjoint on $\mathcal{C}_0^\infty(\mathbb{R}^n)$ and therefore admits a unique **selfadjoint extension** in $\mathcal{H}$ that we call again $\hat{H}$ for simplicity. (example this holds if
Hyp.1 $V \in L^2_{loc}(\mathbb{R}^n)$ and V is real and bounded from below.)

Remark Of course more complicated Hamiltonians can be studied, for example including magnetic potentials, or more singular potentials like Coulomb, or N -body Hamiltonians.

SCHRODINGER Equation

Let ψ be a "wavepacket" at time zero. The wavepacket at time t according to the **quantum evolution** obeys the Schrödinger equation

$$i\hbar \frac{\partial \psi_t}{\partial t} = \hat{H}\psi_t \tag{1.9}$$

with $\psi_0 = \psi$.

Proposition 1.2.2 *Under assumption* **Hyp1** *above, equ. (1.9) admits a unique solution for any $t \in \mathbb{R} \qquad \psi_t \in \mathcal{H}$ given by :*

$$\psi_t = e^{-it\hat{H}/\ \hbar}\psi$$

Here the exponential operator $U_H(t) := e^{-it\hat{H}/\ \hbar}$ is the **unitary** *group in $\mathcal{H}$ generated by the* **selfadjoint** *operator $\hat{H}$ (Stone Theorem)*

Definition 1.2.3 *We shall call* **quantum observable** *any self-adjoint operator in $\mathcal{H}$.*

Definition 1.2.4 *A time-dependent Quantum observable $\hat{A}_t$ is called* **Heiserberg observable** *if it is of the form :*

$$\hat{A}_t := U_H(t)^* \hat{A} U_H(t) \tag{1.10}$$

where $\hat{A}$ is a quantum observable.

Clearly the so- called "Heisenberg representation" (evolution of observables), and the "Schrödinger representation" (evolution of quantum states) are equivalent since, if $\mathcal{D}(\hat{A})$ is invariant under the group $U_H(t)$, for any two states $\varphi, \psi \in \mathcal{D}(\hat{A})$, we have :

$$\langle \varphi, \hat{A}_t \psi \rangle = \langle \varphi_t, \hat{A} \psi_t \ \rangle$$

Definition 1.2.5 *Given two quantum observables $\hat{A}$, $\hat{B}$, with respective domains $\mathcal{D}(\hat{A})$, $\mathcal{D}(\hat{B})$, we define the* **commutator** *of $\hat{A}$, $\hat{B}$*

$$[\hat{A} \ , \ \hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A}$$

defined a priori in the sense of quadratic forms on $\mathcal{D}(\hat{A}) \cap \mathcal{D}(\hat{B})$. It is anti-selfadjoint (under appropriate assumptions on the domains that we shall not make precise here).

Lemma 1.2.6 *Under "appropriate assumptions" on $\hat{A}$, $\hat{H}$ we have :*

$$\frac{d}{dt}\hat{A}_t = \frac{i}{\hbar}[\hat{H} \ , \ \hat{A}_t] \tag{1.11}$$

in a suitable sense (that we shall not make precise here.)

We expect to get a simple correspondence rule between classical and quantum observables. This starts with the so-called **Bohr's prescription**, namely the linear mappings :

$$A \to \hat{A}$$

$$q_j \to \hat{Q}_j$$
$$p_j \to \hat{P}_j$$

where $\hat{Q}_j$ (resp. $\hat{P}_j$) is simply the multiplication operator by x_j (resp. the differential operator $-i\hbar\frac{d}{dx_j}$). These basic operators obey the commutation rule :

$$[\hat{Q}_j \ , \ \hat{P}_k] = i\hbar\delta_{jk}\mathbb{1} \tag{1.12}$$

$\mathbb{1}$ being the identity operator in $\mathcal{H}$. This is called the **Heisenberg incertainty relation**.

1.2.2 Complements on the theory of linear operators in an Hilbert space

In this section $\hat{A}, \hat{B}, \hat{C}$.... denote not necessarily selfadjoint operators in an abstract Hilbert space $\mathcal{H}$. Among “nice” **bounded** operators $\mathcal{B}(\mathcal{H})$, the following are :
-the class of so-called **compact** operators $\mathcal{B}_\infty(\mathcal{H})$
- the class of **trace-class** operators $\mathcal{B}_1(\mathcal{H})$
-the class of **Hilbert-Schmidt** operators $\mathcal{B}_2(\mathcal{H})$

A simple example of trace-class operator is the rank-one projection operator $|\psi\rangle\langle\psi|$.
An example of an operator in $\mathcal{B}_\infty \setminus \mathcal{B}_1$ (and even in $\mathcal{B}_2 \setminus \mathcal{B}_1$) in dimension 1 is simply $(\hat{Q}^2 + \hat{P}^2)^{-1}$.

Definition 1.2.7 *Let $\mathcal{H}$ be a separable Hilbert space, and $\{\varphi_n\}_{n=1}^{\infty}$ any orthonomal basis in $\mathcal{H}$. Than for any* **positive** *$\hat{A} \in \mathcal{B}(\mathcal{H})$ one defines :*

$$tr\hat{A} := \sum_{n=1}^{\infty} \langle\varphi_n, \hat{A}\varphi_n\rangle \tag{1.13}$$

which is a positive number, possibly infinite, and independent of the choice of basis.

Definition 1.2.8 *Let $\hat{B} \in \mathcal{B}(\mathcal{H})$. $\hat{B}^*\hat{B}$ is a selfadjoint positive operator $\in \mathcal{B}(\mathcal{H})$, and one defines $|\hat{B}|$ as*

$$|\hat{B}| := (\hat{B}^*\hat{B})^{1/2} \tag{1.14}$$

which is positive and bounded.

Definition 1.2.9 *$\hat{A} \in \mathcal{B}(\mathcal{H})$ is said to be trace-class (ie $\in \mathcal{B}_1(\mathcal{H})$) if*

$$tr|\hat{A}| < \infty \tag{1.15}$$

Lemma 1.2.10 *$\forall \hat{A} \in \mathcal{B}_1(\mathcal{H})$ one can define*

$$tr\hat{A} = \sum_{n=1}^{\infty} \langle \varphi_n, \hat{A}\varphi_n \rangle \tag{1.16}$$

where $\{\varphi\}_{n=1}^{\infty}$ is an arbitrary orthonormal set (basis) of $\mathcal{H}$. This definition is independent of the chosen basis in $\mathcal{H}$.

Definition 1.2.11 *$\hat{A} \in \mathcal{B}(\mathcal{H})$ is said to be of Hilbert-Schmidt class ($\in \mathcal{B}_2(\mathcal{H})$) if*

$$tr(\hat{A}^*\hat{A}) < \infty \tag{1.17}$$

We then have

$$\|\hat{A}\|_2^2 := tr(\hat{A}^*\hat{A}) = \sum_{m,n=1}^{\infty} |\langle \varphi_n, \hat{A}\varphi_m \rangle|^2$$

for all orthonormal basis $\{\varphi_n\}_{n=1}^{\infty}$ in $\mathcal{H}$

Lemma 1.2.12

$$\mathcal{B}_1 \subset \mathcal{B}_2 \subset \mathcal{B}_\infty \subset \mathcal{B} \tag{1.18}$$

Exercise If $\mathcal{H} = L^2(\mathbb{R}^n)$ and $\hat{A} \in \mathcal{B}_1(\mathcal{H})$ (resp $\in \mathcal{B}_2(\mathcal{H})$) has a "kernel" $K(x, y)$, then
$tr\hat{A} = \int_{\mathbb{R}^n} dx K(x, x)$
(resp $\|\hat{A}\|_2^2 = \int_{\mathbb{R}^{2n}} dxdy |K(x, y)|^2$)

1.2.3 Weyl quantization

When the observables are not simply polynomial functions of $\hat{Q}$, $\hat{P}$, the simple correspondence inherited from the Bohr's prescription has to be made precise. We shall not describe here the **quantization** question in full generality. For more details see :

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Let $f \in \mathcal{S}(\mathbb{R}^{2n})$. One defines the so-called $\hbar$**- Symplectic Fourier Transform** of f as follows :

Definition 1.2.13

$$\widetilde{f}_\hbar(z') := h^{-n} \int_Z dz f(z) e^{i\sigma(z',z)/\hbar} \tag{1.19}$$

Remark : Here and in all that follows one sets as usually in Physics literature

$$h := 2\pi\hbar$$

Exercise : Show that $\widetilde{f}_\hbar \in \mathcal{S}(\mathbb{R}^{2n})$ and

$$f(z) = h^{-n} \int_Z dz' \widetilde{f}_\hbar(z') e^{i\sigma(z,z')/\hbar} \tag{1.20}$$

The idea of Weyl is simply to induce a correspondence by repacing z by $\hat{Z} = (\hat{Q}, \hat{P})$ in equ (1.20) above in the exponential of the symplectic form. One defines :

Definition 1.2.14 *The unitary* **Weyl-Heisenberg translation operators** *are defined by :*

$$\hat{T}(z') := \exp(i\sigma(\hat{Z}, z')/\hbar) = \exp(i(p'.\hat{Q} - q'.\hat{P})/\hbar) \tag{1.21}$$

Exercise Show that

$$\hat{T}(q,0)\psi = \psi(. - q)$$

$$\mathcal{F}(\hat{T}(0,p)\psi) = (\mathcal{F}\psi)(. - p)$$

are simply the operators of translation in coordinate space (resp. momentum space), $\mathcal{F}$ being the Fourier Transform.

Definition 1.2.15 *Given a classical observable $A \in \mathcal{S}(Z)$, we define the* **Weyl quantization** *of A by :*

$$\hat{A} := h^{-n} \int_Z \widetilde{A}_\hbar(z') \hat{T}(z') dz' \tag{1.22}$$

Lemma 1.2.16 *If A is real then its* **Weyl quantization** $\hat{A}$ *is a symmetric (and even selfadjoint) operator.*

Proposition 1.2.17 *The* **Weyl-Heisenberg translation operators** *obey :*
(i)

$$\hat{T}(z)^* = \hat{T}(z)^{-1} = \hat{T}(-z)$$

(ii)

$$\hat{T}(z)\hat{T}(z') = \exp\left(-i\frac{\sigma(z,z')}{2\hbar}\right)\hat{T}(z+z')$$

(iii)

$$\hat{T}(-z)\left(\begin{array}{c}\hat{Q}\\ \hat{P}\end{array}\right)\hat{T}(z) = \left(\begin{array}{c}\hat{Q}+q\\ \hat{P}+p\end{array}\right) = \hat{Z}+z$$

(iv) $\forall\psi \in \mathcal{H}, \quad z = (q,p) \in Z$ *we have :*

$$(\hat{T}(z)\psi)(x) = e^{-ip.q/2\hbar + ip.x/\hbar}\psi(x-q)$$

We leave the proof to the reader as an **exercise**

Proposition 1.2.18 *(i) Let $A \in \mathcal{S}(Z)$ be a classical observable. Then there exists a unique bounded operator $\hat{A} \in \mathcal{B}(\mathcal{H})$ such that $\forall\varphi,\psi \in \mathcal{H}$:*

$$\langle\varphi, \hat{A}\psi\rangle = h^{-n}\int_Z \widetilde{A}_\hbar(z)\langle\varphi, \hat{T}(z)\psi\rangle dz$$

(ii) $\hat{A}\psi$ is given $\forall\psi \in \mathcal{H}$ by the explicit formula

$$(\hat{A}\psi)(x) = h^{-n}\int_Z dydpA(\frac{x+y}{2}, p)\exp(ip.(x-y)/\hbar)\psi(y) \qquad (1.23)$$

(iii) Let $K(x,y) \in \mathcal{S}(\mathbb{R}^{2n})$ be an integral kernel for $\hat{A} \in \mathcal{B}(\mathcal{H})$:

$$(\hat{A}\psi)(x) = \int_{\mathbb{R}^n} K(x,y)\psi(y)dy$$

Then $\hat{A}$ is the Weyl quantization of a **semiclassical symbol** *given by :*

$$A_\hbar(q,p) = \int_{\mathbb{R}^n} K(q+x/2, q-x/2)e^{-ix.p/\hbar}dx$$

In the following we shall make precise the notion of **semiclassical symbol, or observable**, in "nice" classes where the $\hbar$- dependence (for small enough $\hbar$) is sufficiently controlable.

1.2.4 Properties of the Weyl quantization, and semiclassical observables

Definition 1.2.19 *$\gamma = (\gamma_1, \gamma_2 ... \gamma_{2n}) \in \mathbb{N}^{2n}$ is a multiindex*
$A : \mathbb{R}^{2n} \mapsto \mathbb{R}$ is $\mathcal{C}^\infty$ and

$$\frac{\partial^\gamma}{\partial z^\gamma} A = \prod_{k=1}^{2n} \frac{\partial^{\gamma_k}}{\partial z_k^{\gamma_k}} A$$

$$\gamma! := \gamma_1! \gamma_2! ... \gamma_{2n}!$$

$$|\gamma| = \gamma_1 + \gamma_2 + ... \gamma_{2n}$$

A nice class of classical observables is the following :

Definition 1.2.20 *$A \in \mathcal{O}(m)$ $\forall m \in \mathbb{R}$ if $A : Z \mapsto \mathbb{R}$ is $\mathcal{C}^\infty$ and if for all mulitiindex γ, there exists $C > 0$ such that*

$$|\frac{\partial^\gamma}{\partial z^\gamma} A(z)| \leq C(1 + z^2)^{m/2}$$

for all $z = (q, p) \in Z$ $\qquad z^2 = q^2 + p^2$

Lemma 1.2.21 *(i)$\bigcap_m \mathcal{O}(m) = \mathcal{S}(Z)$*
(ii) $\hat{A}^* = \hat{A}$
(iii)$\hat{A}$ is a continuous application $\mathcal{S}(Z) \mapsto \mathcal{S}(Z)$, and $\mathcal{S}'(Z) \mapsto \mathcal{S}'(Z)$ where $\mathcal{S}'$ denotes distributions on $\mathcal{S}$

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The strong link between a classical symbol and its Weyl quantization is expressed in the following result :

Theorem 1.2.22 *Let $\hat{A}$ be the Weyl quantization of a classical symbol A . Then :*
(i)Assume $A \in \mathcal{O}(0)$. Then $\hat{A} \in \mathcal{B}(\mathcal{H})$
(ii) Assume $A \in L^2(Z)$. Then $\hat{A} \in \mathcal{B}_2(\mathcal{H})$ and its Hilbert-Schmidt norm is given by :

$$\|\hat{A}\|_2 = h^{-n/2} \left(\int_Z dz |A(z)|^2 \right)^{1/2}$$

(iii) Assume $A \in \mathcal{O}(m)$ with $m < -2n$. Then $\hat{A} \in \mathcal{B}_1(\mathcal{H})$ and its trace is given by :

$$tr\hat{A} = h^{-n} \int_Z dz A(z)$$

(iv) Assume $A, B \in L^2(Z)$. Then $\hat{A}\hat{B} \in \mathcal{B}_1(\mathcal{H})$ and we have :

$$tr(\hat{A}\hat{B}) = h^{-n} \int_Z dz A(z) B(z)$$

Proof : we shall limit ourselves to (ii)-(iv) the proof of (i) (The Calderon -Vaillancourt Theorem) is more difficult. If $A \in \mathcal{O}(m)$ $\forall m \leq 0$ or $\in L^2(Z)$, then the integral kernel of the operator $\hat{A}$ exists and equals :

$$\hat{A}(x,y) = h^{-n} \int dp A(\frac{x+y}{2}, p) e^{i(x-y).p/\hbar}$$

(ii) If $A \in \mathcal{O}(m)$ for some $m < -2n$, then we have the classical formula :

$$tr\hat{A} = \int_{\mathbb{R}^n} dx \hat{A}(x,x) = h^{-n} \int_Z dx dp A(x,p) \equiv h^{-n} \int_Z A(z) dz$$

(iii)

$$\|\hat{A}\|_2^2 = \int dx dy |\hat{A}(x,y)|^2$$

$$= h^{-2n} \int dx dy | \int dp A(\frac{x+y}{2}, p) e^{i(x-y).p/\hbar}|^2 = h^{-2n} \int du dv | \int dp A(v,p) e^{iu.p/\hbar}|^2$$

$$= h^{-n} \int du dp |A(v,p)|^2$$

using the Plancherel Theorem.

(iv) If $A, B \in L^2(Z)$ then $\hat{A}, \hat{B} \in \mathcal{B}_2(\mathcal{H})$, and thus their product is of trace class.

$$tr(\hat{A}\hat{B}) = \int dx (\int dy \hat{A}(x,y) \hat{B}(y,x)) = \int dx dy \hat{A}(x,y) \hat{B}(y,x)$$

by the Fubini Theorem

$$= h^{-2n} \int dx dy dp dp' A(\frac{x+y}{2}, p) B(\frac{x+y}{2}, p') e^{i(x-y).(p-p')/\hbar}$$

$$= h^{-2n} \int du dv dp dp' A(v,p) B(v,p') e^{iu.(p-p')/\hbar}$$

$$= h^{-n} \int dv dp dp' A(v,p) B(v,p') \delta(p-p') = h^{-n} \int_Z dz A(z) B(z)$$

The above theorem shows that the Weyl quantization establishes a very convenient correspondence between the **classical observables** and the corresponding **quantum observables**, and that the decay properties in phase space of the "classical symbol" imply suitable properties of the quantized observables in the Hilbert space $\mathcal{H}$: bounded, trace-class, Hilbert-Schmidt...

In most applications one considers often **semiclassical observables** (also said "semiclassically admissible") which are the Weyl quantization of entire series in $\hbar$:

$$A_\hbar = \sum_0^\infty \hbar^j A_j$$

where the A_j are classical observables. This appears in particular when one asks the following question :
given $\hat{A}$ $\hat{B}$ the Weyl quantization of two classical symbols A, B, what is the classical symbol corresponding to the product $\hat{C} = \hat{A}\hat{B}$? Since $\hat{A}, \hat{B}$ do not commute, the "classical symbol" of $\hat{C}$ is not a priori real and thus cannot be a classical symbol. It is however a **semiclassical observable** in the following sense :

Definition 1.2.23 *A is a semiclassical observable of weight m (belonging to $\hat{\mathcal{O}}_{sc}(m)$) if it is of the form :*

$$A(\hbar, z) :\asymp \sum_0^\infty \hbar^j A_j(z) \tag{1.24}$$

with $A_j \in \mathcal{O}(m)$ the convergence being true in the following sense :

$$|\frac{\partial^\gamma}{\partial z^\gamma}\left(A(\hbar, z) - \sum_0^N \hbar^j A_j(z)\right)| \leq C_N \hbar^{N+1}(1+z^2)^{N/2}$$

C_N being a constant independent on $\hbar$, z, for any N. A_0 (resp.A_1) are called the **principal** *(resp.* **sub-principal***) symbol. (like in music the fundamental, dominant, sub-dominant tunes...)*

Proposition 1.2.24 *Let $A \in \hat{\mathcal{O}}(m)$ (resp. $B \in \hat{\mathcal{O}}(p)$) ; there exists a unique semiclassical observable $C \in \mathcal{O}(m+p)$ whose Weyl quantization satisfies*

$$\hat{C} = \hat{A}\hat{B}$$

The C_j are given by the formula :

$$C_j = 2^{-j} \sum_{|\alpha+\beta|=j} \frac{(-1)^\beta}{\alpha!\beta!} \left(\frac{\partial^\beta}{\partial q^\beta} \frac{\partial^\alpha}{\partial p^\alpha} A \right) \left(\frac{\partial^\beta}{\partial p^\beta} \frac{\partial^\alpha}{\partial q^\alpha} B \right) \tag{1.25}$$

From the above result, which is simply deduced from simple algebra, we deduce the nice corollary :

Corollary 1.2.25 *Under the assumptions of Prop. (1.2.24), we recover the well-known correspondence between the* **commutator of two quantum observables** *and the* **Poisson bracket of the corresponding classical observables** *:*

$$\frac{i}{\hbar}[\hat{A}\ ,\ \hat{B}] \in \hat{\mathcal{O}}(m+p)$$

and its principal symbol is nothing but $\{A\ ,\ B\}$

Chapitre 2

Coherent States, Squeezed States, Wigner and Husimi Distributions

There exists plenty of families of Coherent States, all relevant to Physics. Among them, some live in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$, others not, some are Gaussian, others not... The more ancient ones come back to Schrödinger himself (1926). For a more detailed and complete review see :

BIBLIOGRAPHY

Perelomov : Generalized Coherent States and their Applications

We shall introduce the Coherent States of the Harmonic Oscillator, which are Gaussian wavepackets that minimize the Heisenberg Uncertainty Relation.

2.1 Coherent States of the Harmonic Oscillator

We have already introduced the operators of translation of Weyl-Heisenberg (equ (1.20)). They monitorize the construction of coherent states, starting from a given wavepacket denoted φ_0 or $|0\rangle$ which is nothing but the ground state of the Harmonic Oscillator. The Hamiltonian of the (isotropic) Harmonic Oscillator is :

$$2\hat{K}_0 := \frac{1}{2}(-\hbar^2\Delta + \hat{Q}^2) \tag{2.1}$$

and its ground state has the following form/

$$\varphi_0(x) := (\pi\hbar)^{-n/4}\exp(-\frac{x^2}{2\hbar}) \tag{2.2}$$

Clearly, when using the following definition of Fourier Transform :

$$\tilde{u}(\xi) := h^{-n/2} \int dx e^{-ix.\xi/\hbar} u(x) \tag{2.3}$$

we have

$$\tilde{\varphi}_0 = \varphi_0$$

and

$$\sigma_{x_k} = \sigma_{p_k} = (\hbar/2)^{1/2}$$

where

$$\sigma_{x_k}^2 := \langle \varphi_0, \hat{Q}_k^2 \varphi_0 \rangle$$

and

$$\sigma_{p_k}^2 := \langle \varphi_0, \hat{P}_k^2 \varphi_0 \rangle$$

for any k between 1 and n, which shows that this wavepacket minimizes the Heisenberg uncertainty relation

$$\sigma_{x_k} \sigma_{p_k} \geq \hbar/2$$

$\hat{T}(z)$ "translates" a wavepacket in phase-space by the vector $z \in Z$. We define the coherent state by :

$$|z\rangle = \hat{T}(z)|0\rangle \tag{2.4}$$

and will note it also by φ_z. Although the "pseudo-support" of φ_0 is localized around the phase-space point 0, the "pseudo-support" of φ_z is localized around z. We shall see later, after introduction of the **"Wigner Transform"** how to give a precise meaning to this assertion.

The usual "creation" and "annihilation" operators $a^\dagger$ and a respectively ($a^\dagger$ is nothing but the adjoint of a in $\mathcal{H}$) are defined as follows :

Definition 2.1.1

$$a := \frac{\hat{Q} + i\hat{P}}{\sqrt{2\hbar}} \qquad a^\dagger := \frac{\hat{Q} - i\hat{P}}{\sqrt{2\hbar}} \tag{2.5}$$

From equ.(1.12) one immediately deduce :

$$[a \ , \ a^\dagger] = \mathbb{1} \tag{2.6}$$

Furthermore we have that φ_0 is in the kernel of a, and more generally that :

Lemma 2.1.2
$$a|z\rangle = \frac{q+ip}{\sqrt{2\hbar}}|z\rangle \tag{2.7}$$
for any $z=(q,p)\in Z$

Proof : it is convenient to introduce compex numbers associated to any $z=(q,p)\in Z$:
$$\alpha := \frac{q+ip}{\sqrt{2\hbar}} \tag{2.8}$$
so that $\hat{T}(z)$ can be rewritten as
$$\hat{T}(z) = e^{\alpha.a^\dagger - \bar{\alpha}.a} \tag{2.9}$$
We shall now make use of the following Baker-Campbell-Haussdorf relation :

Lemma 2.1.3 *If $\hat{A}$, $\hat{B}$ commute with their commutator we have :*
$$e^{\hat{A}+\hat{B}} = e^{-\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{A}}e^{\hat{B}} \tag{2.10}$$
(omitting here the domain considerations of operators for simplicity).

When applied to equ.(2.9) they yield to :
$$\hat{T}(z) = e^{-\frac{|\alpha|^2}{2}}e^{\alpha.a^\dagger}e^{-\bar{\alpha}.a} \tag{2.11}$$
Since $a|0\rangle = 0$ it is easy to show that
$$a|z\rangle = e^{-\frac{|\alpha|^2}{2}}ae^{\alpha.a^\dagger}|0\rangle = e^{-\frac{|\alpha|^2}{2}}[a, e^{\alpha.a^\dagger}]|0\rangle \tag{2.12}$$
and since
$$[a, e^{\alpha.a^\dagger}] = \alpha e^{\alpha.a^\dagger} \tag{2.13}$$
the result follows.

Proposition 2.1.4 *Take any $\psi \in \mathcal{H}$. Then the scalar product $\langle z|\psi\rangle \in L^2(Z)$, and we have :*
$$\int_Z dz|\langle z|\psi\rangle|^2 = h^n\|\psi\|^2 \tag{2.14}$$

2.2 Squeezed States

They are some "cousins" of the coherent states, in the following senses :

-they minimize the uncertainty relations, but instead of having an isotropic profile in phase space they appear to be "squeezed" in some direction, and dilated in the conjugate direction.

-they are "generalized coherent states" in the sense of Perelomov

-whereas the coherent states are monitorized by the Weyl-Heisenberg group which is the exponential of an anti-hermitian **linear** form in $\hat{Q},\ \hat{P}$, the Squeezed States are generated by unitary operators which are antihermitian **quadratic** forms in $\hat{Q},\ \hat{P}$

We shall introduce them here "physically" via the "creation and annihilation" operators introduced above, and restrict ourselves to the case of dimension equal to 1. Then we shall indicate briefly how they can be defined in an equivalent and more general setting via the **metaplectic group** which implements in the "quantum world" the symplectic transformations in canonical classical phase space.

Let β be a complex number of modulus smaller than 1 : $|\beta| < 1$. We define the following complex number :

$$\delta \equiv re^{i\theta} := \frac{\beta}{|\beta|} \tanh^{-1} |\beta| \tag{2.15}$$

$$\hat{S}(\beta) := \exp\left(\frac{1}{2}(\delta a^{\dagger 2} - \bar{\delta} a^2)\right) \tag{2.16}$$

$\delta a^{\dagger 2} - \bar{\delta} a^2$ being antihermitian, $\hat{S}(\beta)$ is unitary and we have :

$$\hat{S}(\beta)^* = \hat{S}(-\beta) \tag{2.17}$$

In terms of operators $\hat{Q}$, $\hat{P}$ of Quantum Mechanics, we have :

$$\hat{S}(\beta) = \exp\left(\frac{i}{2}\Im\delta(\hat{Q}^2 - \hat{P}^2) - \frac{i}{2}\Re\delta(\hat{Q}.\hat{P} + \hat{P}.\hat{Q})\right) \tag{2.18}$$

The **Squeezd States** are thus defined as follows :

Definition 2.2.1

$$\psi_\beta := \hat{S}(\beta)\varphi_0 \tag{2.19}$$

Lemma 2.2.2 *Define* $\gamma := \frac{1-\beta}{1+\beta}$. *We have :*

$$\psi_\beta(x) = \left(\frac{\Re\gamma}{\pi}\right)^{1/4} \left(\frac{1+\bar{\beta}}{|1+\beta|}\right)^{1/2} \exp(-\gamma\frac{x^2}{2}) \tag{2.20}$$

We leave the proof of this lemma and of the important fact that $\Re\gamma > 0$ to the interested reader.

Lemma 2.2.3 *On* $\mathcal{D}(\hat{Q}) \cap \mathcal{D}(\hat{P})$ *we have the following identity :*

$$\hat{S}(\beta)a\hat{S}(-\beta) = (1-|\beta|^2)^{-1/2}(a-\beta a^\dagger) \equiv a\cosh|\delta| - e^{i\theta}a^\dagger \sinh|\delta| \tag{2.21}$$

Indication of the proof : we shall make simply use of the following relation for operators :

$$e^A B e^{-B} = B + \sum_1^n \frac{1}{n!}[A,[A,...[A,B]]]$$

Examples and particular cases

• $\beta \in \mathbb{R},\ 0 < \beta < 1$. Then $\gamma \in \mathbb{R}, \in (0,1)$, thus $\psi_\beta(x)$ is an elongated Gaussian, whereas its Fourier transform $\tilde{\psi}_\beta(\xi)$ is in the contrary a "squeezed Gaussian". Therefore the "phase-space profile" is an elongated ellipse along the q-axis.

• $\forall\beta$ complex, we have a similar picture, but the ellipse is turned by the angle θ. Along the large and small axes of the ellipse, the state ψ_β satisfies :

$$\sigma_q\sigma_p = \frac{\hbar}{2}$$

Important property Consider the following operators :

$$\hat{K}_0 := \frac{a^\dagger.a + a.a^\dagger}{4} \tag{2.22}$$

$$\hat{K}_+ := \frac{1}{2} a^{\dagger 2} \tag{2.23}$$

$$\hat{K}_- := K_+^* = \frac{1}{2} a^2 \tag{2.24}$$

They are simply the generators of Lie -algebra SU(1,1), thus obeying the following commutation rules :

$$[\hat{K}_0, \hat{K}_\pm] = \pm \hat{K}_\pm \tag{2.25}$$

$$[\hat{K}_-, \hat{K}_+] = 2\hat{K}_0 \tag{2.26}$$

We have the following property :

Lemma 2.2.4

$$\hat{S}(\beta)\hat{K}_0\hat{S}(-\beta) = \cosh(2r)\hat{K}_0 - \frac{\sinh(2r)}{2}(\hat{K}_+ e^{i\theta} + \hat{K}_- e^{-i\theta})$$

Following Perelomov (see *BIBLIOGRAPHY*), and the above algebraic properties, one can show that any time dependent Hamiltonian which is **quadratic** in $\hat{Q}$ $\hat{P}$, and therefore of the form :

$$\hat{H}(t) = \lambda(t)\hat{K}_0 + \mu(t)\hat{K}_+ + \bar{\mu}(t)\hat{K}_-$$

(where λ is real) generates via Schrödinger equation a unitary evolution $U(s,t)$ which can be expressed explicitly in terms of $\hat{S}(\beta(t))$ and $\exp(i\hat{K}_0\zeta(t))$, where functions β, ζ can be constructed from λ, μ.
This important property will intervene in a crucial way in the question of "semiclassical" evolution of Coherent States, that will be studied in Chapter 3.

2.3 WIGNER distribution

We shall see in what follows that they are actually **distributions** in the sense put forward by L. Schwartz ; **what Wigner was actually looking for** was an equivalent of the *classical probability distributions* in phase-space Z. That is, associated to any wavepacket (namely a quantum state) a **distribution function** in phase space that **imitates** the classical distribution probability in phase-space.

We recall that a *classical probability distribution* is a **nonnegative** function $\rho \quad : Z \mapsto \mathbb{R}^+$ normalized to unity :

$$\int_Z \rho(z)dz = 1$$

and such that for any classical observable $A \in \mathcal{C}^\infty$, the *mean value* of A in this probability distribution is simply given by

$$\rho(A) \equiv \int_Z dz A(z)\rho(z) \tag{2.27}$$

In the **Quantum world**, given any Observable $\hat{A}$, and any two states $\varphi, \psi \in \mathcal{H}$, the *mean value* of $\hat{A}$ with respect to these states is simply the expectation value $\langle \varphi, \hat{A}\psi \ \rangle$ and one would like to get a distribution

$$(\varphi, \psi) \to W_{\varphi,\psi}(z) \tag{2.28}$$

such that

$$\langle \varphi, \hat{A}\psi \rangle = \int_Z dz A(z) W_{\varphi,\psi}(z) \tag{2.29}$$

for a suitable "distribution" $W_{\varphi,\psi}(z)$ in phase space. Of course it should be antilinear in φ, linear in ψ, and obey (by taking $\hat{A} = \mathbb{1}$) :

$$\int_Z dz W_{\varphi,\varphi} = \|\varphi\|^2 \tag{2.30}$$

In order to proceed to the construction proposed by Wigner, let us come back to a property of the Weyl quantization that we have not written yet.

Lemma 2.3.1 *Let $A \in L^1(\mathbb{R}^n)$. Then its Weyl quantization $\hat{A} \in \mathcal{B}(\mathcal{H})$, and we have :*

$$\|\hat{A}\| \leq (\frac{2}{h})^n \int_Z |A(z)|dz \tag{2.31}$$

Proof :

$$h^n|\langle \psi, \hat{A}\varphi \rangle| = |\int dxdydpA(\frac{x+y}{2}, p)e^{ip.(x-y)/\hbar}\bar{\psi}(x)\varphi(y)|$$

$$= |\int dudvdpA(u,p)\bar{\psi}(u - \frac{v}{2})\varphi(u + \frac{v}{2})e^{iv.p/\hbar}|$$

$$\leq \int dudp|A(u,p)|Sup_{u,p}|\int dv\bar{\psi}(u - \frac{v}{2})\varphi(u + \frac{v}{2})e^{iv.p/\hbar}|$$

$\leq \int dudp|A(u,p)|Sup_u \int dv|\bar{\psi}(u-\frac{v}{2})\varphi(u+\frac{v}{2})| \leq 2^n \int dudp|A(u,p)|\|\psi\|\|\varphi\|$
using Cauchy-Schwarz inequality.

It follows from Lemma (2.3.1) that for any given $\varphi \in \mathcal{H}$, the mapping $W_{\varphi,\varphi} \equiv W_\varphi : A \in \mathcal{S}(Z) \to \langle \varphi, \hat{A}\varphi \rangle \in \mathbb{R}$ via formula (2.29) with $\psi = \varphi$ is a tempered distribution in phase-space Z. Thus formula (2.29) is the defining equation for the **Wigner distribution** associated to the pair $(\psi, \varphi) \in \mathcal{H}$. We have the following :

Lemma 2.3.2 *(i)We have $W_{\varphi,\psi} \in L^\infty(Z)$ and it can be written as*

$$W_{\varphi,\psi}(q,p) = h^{-n} \int_{\mathbb{R}^n} dy \bar{\varphi}(q+\frac{y}{2})\psi(q-\frac{y}{2})e^{ip.y/\hbar} \tag{2.32}$$
$$= h^{-n} \int_Z dz \langle \varphi, \hat{T}(z)\psi \rangle e^{i\sigma(z,z')/\hbar}$$

(ii) $h^n W_{\varphi,\psi}(z)$ is the Weyl symbol for the rank one operator $|\psi\rangle\langle\varphi|$.

Proof : (i) We use the definition (1.2 15) of the Weyl quantization of a symbol A :

$$\langle \varphi, \hat{A}\psi \rangle = h^{-n} \int dxdydpA(\frac{x+y}{2}, p)e^{i(x-y).p\hbar}\bar{\varphi}(x)\psi(y)$$

so that performing the change of variables (of Jacobian 1) $x - y = u$, $\frac{x+y}{2} = v$, we get :

$$\langle \varphi, \hat{A}\psi \rangle = \int dpdqA(q,p)h^{-n} \int dv e^{ip.u/\hbar}\bar{\varphi}(q+\frac{v}{2})\psi(q-\frac{v}{2}) \tag{2.33}$$
$$= \int_Z dpdqA(q,p)W_{\varphi,\psi}(q,p)$$

or in other words,

$$\langle \varphi, \hat{A}\psi \rangle = h^{-n} \int_Z dz \widetilde{A}_\hbar(z) \langle \varphi, \hat{T}(z)\psi \rangle$$

We now use the Plancherel Theorem for the symplectic-Fourier Transform $f \to \tilde{f}_\hbar$:

$$= \int_Z dz' A(z') W_{\varphi,\psi}(z')$$

where

$$W_{\varphi,\psi}(z') := h^{-n} \int dz \langle \varphi, \hat{T}(z)\psi \rangle e^{-i\sigma(z',z)/\hbar}$$

(ii) Clearly, if $\Pi_{\varphi,\psi} := |\psi\rangle\langle\varphi|$, and if $A \in \mathcal{S}(Z)$ we get :

$$\langle\varphi, \hat{A}\psi\rangle = tr(\hat{A}\Pi_{\varphi,\psi}) \equiv h^{-n}\int_Z dz A(z)B(z)$$

where B is the "Weyl symbol" of $\Pi_{\varphi,\psi}$, where we have used Theorem 1.2.22 (iv). We then identify $h^n W_{\varphi,\psi}$ as the Weyl symbol of $\Pi_{\varphi,\psi}$.

Question : What about the expected properties of $W_{\varphi,\psi}$ as a possible probability distribution in phase-space ?, namely :

-positivity
-normalization to 1
- correct marginal distributions ?

Lemma 2.3.3 *Let $z = (q,p) \in Z$, $\varphi \in \mathcal{H}$, $\|\varphi\| = 1$. We have :*

(i)

$$\int_{\mathbb{R}^n} dp W_\varphi(q,p) = |\varphi(q)|^2 \tag{2.34}$$

= probability amplitude to find the quantum particle at position q

(ii)

$$\int_{\mathbb{R}^n} dq W_\varphi(q,p) = |\mathcal{F}\varphi(p)|^2 \tag{2.35}$$

= probability amplitude to find the quantum particle at momentum p

(iii)

$$\int_Z dq dp W_\varphi(q,p) = 1 \tag{2.36}$$

(iv) $W_\varphi(z) \in \mathbb{R}$
(v) $W_\varphi(z) \geq 0 \iff \varphi$ is Gaussian, but can take negative values if φ is not.

Proof of (i). Let $f \in \mathcal{D}$ be an arbitrary test function. We have :

$$\int_{\mathbb{R}^n} W_\varphi(q,p) f(p) dp = h^{-n}\int dy \bar{\varphi}(q+\frac{y}{2})\varphi(q-\frac{y}{2})\int dp e^{ip.y/\hbar} f(y)$$

$$\int dy \bar{\varphi}(q+\frac{y}{2})\varphi(q-\frac{y}{2})(\mathcal{F}f)(y)$$

By taking for $\mathcal{F}f$ an approximation of the Dirac distribution in $y = 0$, we get the result. The proof of (ii) is similar, and the proof of (iii) follows immediately.
The proof of (iv)-(v) is left to the reader as an **exercise**.

Lemma 2.3.4 *Let $a > 0$ and ψ the normalized Gaussian wavefunction*

$$\psi(x) = (\frac{\pi\hbar}{a})^{-n/4} e^{-ax^2/2\hbar}$$

Then we have :

$$W_\psi(q,p) = (\pi\hbar)^{-n} \exp(-(aq^2 + \frac{p^2}{a})/\hbar) \tag{2.37}$$

The proof is an easy calculus that we leave to the reader.

If $a = 1$ then $\psi = |0\rangle$ is the coherent state centered at 0, and its Wigner function is an isotropic Gaussian centered in 0, which corroborates the assertion that its "pseudo-support" is a ball of radius $\sqrt{\hbar}$.

If $a \neq 1$ then ψ is a "squeezed state", and the profile in phase-space is an ellipse.

Proposition 2.3.5 *Let φ, ψ be quantum states $\in L^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$. Then $W_{\varphi,\psi} \in L^2(Z) \cap L^\infty(Z)$ and we have :*

$$\|W_{\varphi,\psi}\|_{L^\infty} \leq (\frac{2}{\hbar})^n \|\varphi\|_2 \|\psi\|_2 \tag{2.38}$$

and

$$\|W_{\varphi,\psi}\|_{L^2} \leq h^{-n/2} \|\varphi\|_2 \|\psi\|_2 \tag{2.39}$$

The proof of equ. (2.38) is a simple consequence of Lemma 3.2.2 (equ. (2.32)). Let us now check equ. (2.39).

$$\int_Z dz |W_{\varphi,\psi}(z)|^2 = h^{-2n} \int dqdp |\int dy e^{ip.y/\hbar} \bar{\varphi}(q + \frac{y}{2}) \psi(q - \frac{y}{2})|^2$$

But $\bar{\varphi}(q+\frac{y}{2})\psi(q-\frac{y}{2}) \in L^2(\mathbb{R}^n, dy)$ so that via Plancherel Theorem we get :

$$h^{-n}\int dp|\int dy\bar{\varphi}(q+\frac{y}{2})\psi(q-\frac{y}{2})|^2 = \int dy|\bar{\varphi}(q+\frac{y}{2})\psi(q-\frac{y}{2})|^2$$

Moreover the RHS $\in L^2(\mathbb{R}^n, dq)$, and therefore

$$\|W_{\varphi,\psi}\|_2^2 = h^{-n}\int dqdy|\bar{\varphi}(q+\frac{y}{2})\psi(q-\frac{y}{2})|^2 = h^{-n}\|\varphi\|^2\|\psi\|^2$$

which completes the proof of the Proposition.

Proposition 2.3.6 *Let $\varphi,\ \psi$ be quantum states $\in L^2(\mathbb{R}^n)\cap L^\infty(\mathbb{R}^n)$ and let $W_\varphi,\ W_\psi$ be the associated Wigner functions. We have :*

$$|\langle\varphi,\psi\rangle|^2 = h^n(W_\varphi, W_\psi)_{L^2(Z)} \tag{2.40}$$

The Wigner Transformation operates "as one wishes" in phase-space, ie according to the scheme of classical mechanics :

Proposition 2.3.7 *Let $\varphi,\ \psi \in \mathcal{H}$, and $\hat{T}(z),\ \hat{R}(M)$ be respectively operators of the Weyl-Heisenberg and metaplectic group, corresponding respectively to*
-a phase-space translation by vector z
-a symplectic tranformation in phase-space.

We have :

$$W_{\hat{T}(z')\varphi,\hat{T}(z')\psi}(z) = W_{\varphi,\psi}(z-z') \tag{2.41}$$

$$W_{\hat{R}(M)\varphi,\hat{R}(M)\psi}(z) = W_{\varphi,\psi}(Mz) \tag{2.42}$$

Proof : We start from formula (2.32) (second line) and

$$\hat{R}(M)^{-1}\sigma(\hat{Z},z)\hat{R}(M) = \sigma(M^{-1}\hat{Z},z) = \sigma(\hat{Z},Mz)$$

so that :

$$W_{\hat{R}(M)\varphi,\hat{R}(M)\psi}(z) = h^{-n}\int du\langle\varphi,\hat{T}(Mu)\psi\rangle e^{i\sigma(z,Mu)/\hbar} = W_{\varphi,\psi}(Mz)$$

We end this section by an important result about **coherent states** :

Proposition 2.3.8 *Let $|z\rangle$ be a coherent state; then $\forall A \in \mathcal{S}(Z)$ we have*

$$\lim_{\hbar\to 0}\langle z|\hat{A}|z\rangle = A(z) \tag{2.43}$$

Proof : We have seen that $W_{\varphi_0} = (\pi\hbar)^{-n}e^{-(q^2+p^2)/\hbar}$, and similarly

$$W_{\varphi_z}(q',p') = \exp\left(-\frac{(q-q')^2}{\hbar} - \frac{(p-p')^2}{\hbar}\right)$$

But $W_{\varphi_z} \to \delta(z-z')$ in distributional sense, which yields the result.

Physical Interpretation : The coherent states are those quantum states which are at most localized in phase space around a given point in a ball of radius $\sqrt{\hbar}$. The classical symbol of an operator $\hat{A}$ is nothing but the classical limit $\hbar \to 0$ of the expectation value $\langle z|\hat{A}|z\rangle$ of $\hat{A}$ in the coherent state.

2.4 Husimi Distribution, and Anti-Wick Quantization

The **coherent states** are also often used in order to define another quantization of classical observables, called **Anti-Wick quantization** in the physical literature (and Berezin or Toeplitz in the mathematical one.) Alike Weyl quantization, it associates to a classical observable (**real**) a quantum one (**selfadjoint**), but it in addition preserves the positivity as we shall see.

Definition 2.4.1 *Let $A \in \mathcal{S}(Z)$ be a classical observable. One defines its anti-Wick quantization $\check{A}$ as*

$$\check{A} := \int_Z dz A(z)|z\rangle\langle z| \tag{2.44}$$

Lemma 2.4.2 *If $A(z) \geq 0$, then $\check{A} \geq 0$ (in the sense of quadratic forms).*

Proof : obvious since

$$\forall\psi \in \mathcal{H}, \qquad \langle\psi, \check{A}\psi\rangle = \int_Z dz A(z)|\langle\ \psi|z\rangle|^2 \geq 0$$

Proposition 2.4.3 *For all $A \in \mathcal{O}(0)$ a classical observable (real), its anti-Wick quantization $\check{A}$ is a bounded selfadjoint operator in $\mathcal{H}$ (as the Weyl quantization $\hat{A}$).*

Proof : $\forall \varphi,\ \psi \in \mathcal{H}$ we have :

$$\langle \varphi, \check{A}\psi \rangle = \int_Z dz A(z) \langle z|\psi\rangle \langle \varphi|z\rangle$$

Thus :

$$|\langle \varphi, \check{A}\psi \rangle| \leq \|A\|_{L^\infty(Z)} \int_Z dz |\langle z|\psi\rangle \langle \varphi|z\rangle|$$

$$\leq \|A\|_{L^\infty(Z)} \left(\int_Z |\langle z|\psi\rangle|^2\right)^{1/2} \left(\int_Z dz |\langle z|\varphi\rangle|^2\right)^{1/2} \leq h^n \|A\|_{L^\infty(Z)} \|\psi\| \|\varphi\|$$

Therefore $\|\check{A}\psi\| \leq h^n \|A\|_{L^\infty(Z)} \|\psi\|,\ \forall \psi \in \mathcal{H}$

The **coherent states** (sometimes called continuous overcomplete basis of $\mathcal{H}$) are also very useful to calculate the Trace of an operator :

Proposition 2.4.4 *Let $\hat{A} \in \mathcal{B}_1(\mathcal{H})$ be a (not necessarily selfadjoint) trace-class operator . Then we have*

$$tr\hat{A} = h^{-n} \int_Z dz \langle z|\hat{A}|z\rangle \tag{2.45}$$

The proof is left to the reader, who may use the integral kernel of $\hat{A}$: $\hat{A}(x, y)$, the formula $tr\hat{A} := \int_{R^n} \hat{A}(x, x)$ and the formula :

$$\varphi_z(x) = (\pi\hbar)^{-n/4} \exp\left(-\frac{ip.q}{2\hbar} + \frac{ip.x}{\hbar} - \frac{1}{2\hbar}(x-q)^2\right) \tag{2.46}$$

Finally the **coherent states** are useful to define a "regularization" of the Wigner distribution, called the **Husimi distribution**, and noted H_ψ, which to any quantum state ψ associates $H_\psi :\ Z \mapsto \mathbb{R}^+$. Since it is non-negative, it is a better candidate than the Wigner distribution to "imitate" a classical probability distribution.

Definition 2.4.5 *The Husimi distribution associated to any $\psi \in \mathcal{H}$ is :*

$$H_\psi(z) := h^{-n} |\langle z|\psi\rangle|^2 \tag{2.47}$$

In fact $H_\psi(z)$ is nothing but a "regularization" of the Wigner distribution : since

$$|\langle z|\psi\rangle|^2 = h^n (W_{\varphi_z}, W_\psi)_{L^2(Z)}$$

and $W_{\varphi_z}(z') = \Psi_0(z'-z)$ where $\Psi_0(z)$ is the normalized Gaussian

$$\Psi_0(z) = (\pi\hbar)^{-n} e^{-z^2/\hbar} \tag{2.48}$$

of L^1 norm equal to 1 we deduce :

$$H_\psi = W_\psi * \Psi_0$$

In the following pages we present a comparative tableau of the Classical Mechanics, and Quantum Mechanics notions, recapitulating the two previous Chapters.

CLASSICAL WORLD	QUANTUM WORLD
$Z = \mathbb{R}^n \times \mathbb{R}^n$ PHASE SPACE	$\mathcal{H} = L^2(\mathbb{R}^n)$ Hilbert space of quantum states
$z := (q, p)$ classical state of a particle	$\varphi \in \mathcal{H}$ "wavefunction"
q : position or coordinate	$\hat{Q}$
p : momentum	$\hat{P} := -i\hbar\nabla$ self-adjoint Operators
Hamiltonian $H = \frac{p^2}{2m} + V(q)$	Quantum **Hamiltonian** $\hat{H} := -\frac{\hbar^2}{2m}\Delta + V(q)$
Real	Self-Adjoint
Phase-Space Evolution : $(q, p) \to (q_t, p_t) = \phi^t_H(q, p)$	**Quantum evolution** : $U_H(t) := e^{-it\hat{H}/\hbar}$
ϕ^t_H preserves Phase-Space volumes	Unitary Operator
Classical Observables	**Quantum Observables**
$A : Z \mapsto \mathbb{R}$	$\hat{A}$: Weyl Quantization of A
Evolution of classical Observables	**Evolution of Quantum Observables**
$A \circ \phi^t_H$	$\hat{A}_t := U^*_H(t)\hat{A}U_H(t)$
Geometrical Tranformations	**Unitary Transformations in $\mathcal{H}$**
• Phase-space translations	• $\hat{T}(z) := \exp(i\hat{Z}.Jz/\hbar)$ Weyl-Heisenberg operator

CLASSICAL WORLD (continued)

•, $J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}$ represents rotations of $\frac{\pi}{2}$

• General **symplectic** tranformations, ie

Preserve symplectic form
$\sigma(z, z') = z.Jz'$

M : **symplectic matrix** $2n \times 2n$

Example $M = \begin{pmatrix} e^{\gamma}\mathbb{1} & 0 \\ 0 & e^{-\gamma}\mathbb{1} \end{pmatrix}$
dilation/squeezing transformation

Multiplicative Group :
$M = M_1 M_2$ symplectic

CLASSICAL STATE
Point $z \in Z$

Probability Distribution in PHASE SPACE :

$f: \; Z \mapsto \mathbb{R}^+$

QUANTUM WORLD (continued)

• $\mathcal{F}$ Fourier Transformation

• General operators of **metaplectic** Group

$i\sigma(\hat{Z}, z)$ generator of Weyl-Heisenberg Group

$B: \; 2n \times 2n$ real symmetric
$M = e^{JB} \to \hat{R}(M) = e^{i\hat{Z}.B\hat{Z}/2\hbar}$

$\hat{D}(\gamma) := \exp \frac{i\gamma}{2\hbar}(\hat{Q}.\hat{P} + \hat{P}.\hat{Q}))$

$\hat{R}(M_1 M_2) = \hat{R}(M_1)\hat{R}(M_2)$ is **Group**

COHERENT STATE $|z\rangle$

WIGNER, HUSIMI distributions

$\varphi \in \mathcal{H}, \; \|\varphi\| = 1$

CLASSICAL WORLD (continued)	QUANTUM WORLD (continued)
	Wigner Distribution
	$\to W_\varphi(q,p)$ **not** ≥ 0 in general
	Husimi Distribution
$f(q,p) \geq 0$	$H_\varphi(z) := \vert\langle\varphi\vert z\rangle\vert^2 \geq 0$
$\int_Z f(z)dz = 1$	$\int_Z dz W_\varphi(z) = \int_Z dz H_\varphi(z) = 1$

Chapitre 3

Semiclassical Propagation

One wants to study in which respect Bohr is right when he proposes his famous **correspondence principle** which can be paraphrased in the following way :
when the Planck constant $\hbar$ is small as compared with a classical action characteristic of the system, the Quantum Theory approaches the Classical Newton's Theory.

But, letting $\hbar$ tend to zero in the equations of Quantum Mechanics is a limit mathematically very singular, as we'll show it ; and in particular the limit $\hbar \to 0$ **doesn't commute** with the limit $t \to \infty$, which is the limit in which the properties of being possibly ergodic, hyperbolic, or "chaotic" of the classical mechanics manifest themselves.

It is thus useful to study in detail this **semiclassical** limit, precisely in link with the propagation in time properties of the system (semiclassical dynamics or propagation).

In the seventies, Maslov and Hörmander introduced (independently) a new tool particularly efficient, called **microlocal analysis**, which allows to construct approximations of the Quantum Propagators via a class of operators called Fourier-Integral-Operators. We shall sketch rapidly this approach in Section 2, in link with the so called **WKB method** very famous among physicists.

In the first Section we shall study more precisely the semiclassical propagation of observables (Egorov Theorem), whereas Section 3 will be devoted to the semiclassical propagation of the coherent states. These last properties will be particularly powerful in a rigorous approach of so-called "quantum chaos problems" that will be introduced in Chapter 5.

3.1 Semiclassical Evolution of Observables

BIBLIOGRAPHY

Egorov : On canonical transformations of pseudodifferential operators

Theorem 3.1.1 *Let H be a semiclassical Hamiltonian $\in \mathcal{O}_{sc}(2)$ satisfying*

$$|\partial_z^\gamma H_j(z)| \leq C_\gamma \qquad |\gamma| + j \geq 2 \tag{3.1}$$

$$\hbar^{-2}(H - H_0 - \hbar H_1) \in \mathcal{O}_{sc}(0) \tag{3.2}$$

and let A be a classical observable $\in \mathcal{O}(m)$ for some $m \in \mathbb{R}$. We have :

(i) For sufficiently small $\hbar$, $\hat{H}$ is essentialy-selfadjoint on $\mathcal{S}(\mathbb{R}^n)$ and therefore the quantum evolution operator

$$U_H(t) := \exp(-it\hat{H}/\hbar)$$

is unitary in $\mathcal{H}$ $\qquad \forall t \in \mathbb{R}$

(ii)$\forall t \in \mathbb{R},\ \hat{A}(t) := U_H(t)^* \hat{A} U_H(t) \in \mathcal{O}_{sc}(m)$
Its semiclassical symbol has the following asymptotic expansion :

$$A(t) \asymp \sum_{j\geq 0} \hbar^j A_j(t) \qquad A_j \in \mathcal{O}(m)$$

uniformly in $t \in [-T, T]$

$$A_0(t, z) = A(\phi^t_{H_0}(z))$$

$$A_1(t, z) = \int_0^t ds \left\{A \circ \phi^s_{H_0}, H_1\right\} \phi^{t-s}_{H_0}(z)$$

and a general explicit formula can be written for $A_j(t, z)$ $\qquad \forall j \geq 2$

Note that the **classical dynamics** involved in this semiclassical expansion is that induced by **the principal symbol** H_0 of H. Under the assumptions of Theorem (3.1) the classical flow $\phi^t_{H_0}$ exists globally in time. Namely the vector field $(\partial_p H_0, -\partial_q H_0)$ has a sub-linear increase at ∞, therefore no classical trajectory can blow up in finite time.

Moreover one can show that $A\circ\phi^t_{H_0} \in \mathcal{O}(m)$ with the seminorm in $\mathcal{O}(m)$ uniformly bounded for $t \in [-T, T]$. We use the following notations :

$$A_0(t,z) := A \circ \phi_{H_0}(z) \tag{3.3}$$

$\widehat{A_0}(t)$ is the Weyl quantization of $A_0(t,z)$.
Using the evolutions equations for H_0 and $\hat{H}_0$ respectively, we get :

$$\frac{d}{dt}U_H(-s)\widehat{A_0}(t-s)U_H(s) = U_H(-s)\left(\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \{\widehat{H_0, A_0}\}\phi^{t-s}_{H_0}\right)U_H(s) \tag{3.4}$$

We have seen (corollary 1.2.25) that the principal symbol of $\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)]$ is $\{H_0, A_0(t-s)\}$ and therefore the principal symbol of the RHS of (3.4) is zero. By integrating (3.4) in s from 0 to t, we get :

$$U_H(t)^*\hat{A}U_H(t) - \widehat{A_0}(t) = O(\hbar)$$

By induction we obtain in this way the successive terms of the semiclassical expansion of $\hat{A}(t)$.

Corollary 3.1.2 *We call φ_z a coherent state. Then for any observable $A \in \mathcal{O}(m)$ and all Hamiltonian as in Theorem 3.1, we have :*

$$\lim_{\hbar\to 0}\langle U_H(t)\varphi_z, \hat{A}U_H(t)\varphi_z\rangle = A \circ \phi^t_{H_0}(z) \tag{3.5}$$

uniformly for $y \in [-T, T]$

Proof : since $\varphi := \hat{T}(z)\varphi_0$we have :

$$\langle U_H(t)\varphi_z, \hat{A}U_H(t)\varphi_z\rangle = \langle \varphi_0, \hat{T}(-z)U_H(t)^*\hat{A}U_H(t)\hat{T}(z)\varphi_0\rangle$$

so that if we denote as usual $\Pi_0 := |0\rangle\langle 0|$ the projector on $\varphi_0 = |0\rangle$ the RHS of equation above is nothing but

$$tr\Pi_0\hat{T}(-z)U_H(t)^*\hat{A}U_H(t) = \int_Z dz' W_{\varphi_0}(z')B_{t,z}(z')$$

where $B_{t,z}$ is the Weyl symbol of the operator$\hat{T}(-z)U_H(t)^*\hat{A}U_H(t)\hat{T}(z)$. But the principal symbol has been shown to be :

$$A \circ \phi^t_{H_0}(z+z')$$

Therefore, using the explicit Gaussian formula for W_{φ_0} we get :

$$\lim_{\hbar\to 0}\langle U_H(t)\varphi_z, \hat{A}U_H(t)\varphi_z\rangle = \lim_{\hbar\to 0}(\pi\hbar)^{-n}\int_Z dz' e^{-z'^2/\hbar}(A\circ\phi^t_{H_0})(z+z') = A\circ\phi^t_{H_0}(z)$$

This therefore generalizes to the case of semiclassical time-dependent observables the result ot Proposition 2.3. 8 :

The Heisenberg Observable $U_H(t)^*\hat{A}U_H(t) \to A\circ\phi_{H_0}$ dyn. Class. Observable as $\hbar \to 0$,
H_0 being the principal symbol of H.

3.2 WKB method / Microlocal Analysis

3.2.1 Reminders

The WKB approximation consists in looking for an integral Representation of a quatum state $\psi_\hbar(x) \in \mathcal{S}'(\mathbb{R}^n)$ of the following form :

$$\psi_\hbar(x) = \int_\Theta d\theta e^{i\Phi(x,\theta)/\hbar} A(\hbar, x, \theta) \tag{3.6}$$

Θ being an Euclidean space called "frequency variables set", Φ being a **real phase**, and A a **complex amplitude** of the following form :

$$A(\hbar, x, \theta) \asymp \sum_{j\geq 0} \hbar^j A_j(x,\theta) \tag{3.7}$$

$\psi_\hbar$ can also be the integral kernel of a quantum Observable or of a quantum Propagator ; let, say, $K(\hbar, t; x, y)$ be the integral kernel of $U_H(t)$. It obeys :

$$i\hbar\frac{\partial}{\partial t}K(\hbar, t; x, y) = (\hat{H}K(\hbar, t; ., y))(x) \tag{3.8}$$
$$K(\hbar, 0; x, y) = \delta(x-y)$$

In fact equ.(3.6) and (3.7) can be interpreted as a particular class of so-called **Fourier Integral Operators**, whose prototype is the well-known Fourier representation of Dirac distributions :

$$\delta(x-y) = h^{-n}\int_{\mathbb{R}^n} e^{i(x-y).\eta/\hbar} d\eta$$

The study of **Fourier Integral Operators** together with that of **Pseudo-Differential Operators** is an important branch of mathematics, more precisely of the Microlocal Analysis. We shall here, without entering the whole complexity of the Fourier Integral Operators "machinery", sketch rapidly which sense can be attributed to expressions like (3.6). Then we shall focus on the application of this scheme to an approximation of $K(\hbar, t; x, y)$.

3.2.2 Fourier Integral Operators, a brief sketch

Note by $T(\Phi, A, \hbar)$ the distribution defined by equ. (3.6) :

$$(T(\Phi, A, \hbar), f) := \int_{\Theta\times X} dx d\theta e^{i\Phi(x,\theta)/\hbar} A(\hbar, x, \theta) f(x) \qquad \forall f \in \mathcal{S}(X) \quad (3.9)$$

Note that regularity assumptions are necessary on Φ and A and also on their decrease at infinity, in order to study their properties, together with an assumption of the form :

$$\exists C > 0 \quad : \ C^{-1}\|(x,\theta)\| \leq \|\nabla\Phi.x\| \leq C\|(x,\theta)\| \qquad (3.10)$$

Here $\|z\| := (1+z^2)^{1/2}$ which **is not a norm**. We can then attribute a sense to distributions T by the method of **stationary phase** ie by estimating the highly oscillatory integral (3.9) at points where $\nabla\Phi(x,\theta) \neq 0$. We then have

Definition 3.2.1 *An FIO operator is a mapping defined on $\mathcal{S}(X)$ by :*

$$I(\Phi, A, \hbar) f(x) := \int_{\Theta\times X} d\theta dy e^{i\Phi(x,\theta,y)/\hbar} A(\hbar, \theta, x, y) f(y) \qquad (3.11)$$

Under suitable assumptions on Φ, A this defines a mapping of $\mathcal{S}(X)$ into itself, and the product ot two FIO is a FIO.

3.2.3 Applications to the semiclassical approximation of the quantum Propagator

For quantum Hamiltonians $\hat{H} = -\hbar^2\Delta + V$ acting in $\mathcal{H}$, with regular potentials growing at most quadratically at infinity, we look for semiclassical expansions of K of the form :

$$K(\hbar, t; x, y) = h^{-n} \int_{X^*} dp e^{i(S(t,x,p)-y.p)/\hbar} \sum_{j\geq 0} \hbar^j A_j(t, x, p) \tag{3.12}$$

with initial data (t=0) :

$$S(0, x, p) = x.p$$

$$A_0(0, x, p) = 1$$

$$A_j(0, x, p) = 0 \quad j \geq 1 \tag{3.13}$$

Due to Schrödinger equation (3.8), and reporting the expansion (3.12) we get, at least fomally :

$$\partial_t S(t, x, p) + H(x, \nabla_x S(t, x, p)) = 0 \tag{3.14}$$

$$S(0, x, p) = x.p$$

which is **Hamilton-Jacobi** equation , together with **transport equations** which we shall not write explicitly here.

Theorem 3.2.2 *Let $\hat{H}$ be the Weyl quantization of a semiclassical Hamiltonian satisfying assumptions ot Egorov's Theorem. Then $\exists T > 0$ small enough such that :*

(i)The Hamilton-Jacobi equation (3.14) has a unique solution $S(t, x, p)$ $\forall |t| < T$ which is the generating function of the classical flow for H :

$$\phi_H^t(x, \partial_x S(t, x, p)) = (\partial_p S(t, x, p), p) \tag{3.15}$$

(ii)The transport equations define by induction the A_j's in a unique way $\in \mathcal{C}^\infty([-T, T] \times Z)$ such that :

$$|\partial_t^k \partial_z^\gamma A_j(t, z)| \leq C_{k,\gamma} \quad \forall k \in \mathbb{N},\ \gamma \in \mathbb{N}^{2n} \tag{3.16}$$

uniformly in $[-T, T] \times Z$.
(iii) $\forall N \in \mathbb{N}$, *the FIO defined for* $t \in [-T, T]$ *:*

$$U_{H,N}(t)\varphi(x) = h^{-n} \int_Z dpdy e^{i(S(t,x,p)-y.p)/\hbar} \sum_0^N \hbar^j A_j(t,x,p)\varphi(y) \tag{3.17}$$

is bounded in $\mathcal{H}$ *and is a good approximation of the quantum propagator :*

$$Sup_{|t|\leq T} \|U_H(t) - U_{H,N}(t)\|_{\mathcal{B}(\mathcal{H})} = O(\hbar^N) \tag{3.18}$$

The particular form of the FIO :

$$\int_Z dyd\eta e^{(S(t,x,\eta)-y.\eta)/\hbar} A_j(t,x,\eta)\varphi(y)$$

allows one to make use of suitable "Calderon-Vaillancourt -type" Theorems so that the FIO is bounded in $\mathcal{H}$, for the given S and A_j's, for t small enough. However this proof is far from being trivial and we'll skip it, and don't enter further into this "machinery", prefering the method based on coherent states which is closer to the physical intuition.

Moreover the fact that we are restricted to small values of t comes from the fact that the FIO representation encounters **caustic problems**. We shall briefly present these caustics in the following subsection.

3.2.4 What are Caustics ?

We have seen that the WKB approximation (which actually goes back to Liouville, Green, Stokes and Rayleigh) allows an "imitation" of the passage in physics optics of the propagation of light as an electromagnetic wave to its propagation in terms of rays (geometrical optics). As in geometrical optics, this description - as an approximation when the wavelength is short compared to the dimension of material bodies it encounters - presents physical and mathematical limitations known as "caustics". This term is inherited from the geometrical optics where it represents the **envelope of the family of rays** : they can be visualized on a wall lighted par rays diffracted by a smooth surface.

One can show that the phase of wave oscillations along a given ray has a **discontinuity** (of one quarter of wavelength) when passing through the caustic.

We suall indicate more precisely what are caustics in the semiclassical limit in order to better understand how to overcome the mathematical problems they introduce.

see *BIBLIOGAPHY*
Arnold : Méthodes Mathématiques de la Mécanique Classique

Assume the initial solution of the Schrödinger equation be of the following form :

$$\psi(q) := A(q)e^{iS(q)/\hbar}$$

We associate to our initial data a **Lagrangian manifold** in phase-space, namely a manifold of dimension n on which the symplectic form $dq \wedge dp$ on Z is identically zero :

$$p(q) := \nabla S(q) \tag{3.19}$$

is the momentum corresponding to our initial condition.

Lemma 3.2.3 *For all differentiable function $q \to S(q) \ \in \mathcal{C}^1(\mathbb{R}^n)$ the graph of the function $p(q)$ above is a* **Lagrangian manifold***. Conversely if a Lagrangian Manifold projects itself in an unique way on the configuration space $\mathbb{R}^n$, (namely is a graph), then it is defined by a genaration function via formula (3.19)*

If M is a Lagrangian Manifold for some initial condition of the form above, then for t not too large the classical flow ϕ_H^t transforms it into $\phi_H^t M$ which is again Lagrangian. This is no longer true in general if t becomes large. The points of $\phi_H^t M$ which project to some $Q \in \mathbb{R}^n$ are images by ϕ_H^t of in general several points of M. In other terms at point Q terminate two or more trajectories of the classical particle whose initial data lie on M. The points where the tangent plane to the manifold is of the form q = cst are singular points. The set of such points form by projection on configuration space an apparent contour called **Caustic**. To these points are associated **integer indices** called Morse indices which are the semiclassical analogues of the discontinuity of the phase in going from wave optics to geometrical optics. These indices will play an important rôle in the Trace Formulae that will be studied in Chapter 5.

Summary

A Lagrangian manifold is a manifold in phase-space Z generated by $S(q, p, t)$. At some points $q = Q$ there may have two different trajectories of the classical flow ϕ_H^t for initial data on some initial Lagrangian manifold M. This generates so-called "caustic problems" that can be avoided, starting from a "good" M by letting t to be small enough so that this doesn't occur.

Thus the "caustics problems" appear if one wants to **project** the Lagrangian manifold $\phi_H^t M$ on configuration space when t becomes large. They can however be **avoided** if one works **entirely in phase-space** for the Quantum Propagator. We do precisely this by studying the semiclassical propagation of **coherent states.**

3.3 Semiclassical Propagation of Coherent States

In order to circumvent the limitation to small times introduced by caustic problems, we work entirely in phase space. For doing this, a good idea is to use the coherent states which, as we have shown above, "imitate " at most as possible classical points in phase-space, at least in the semiclassical limit. (Their Wigner function, gaussian and nonnegative is localized around a phase space point in a ball if radius $\sqrt{\hbar}$).

Along a tradition which goes back to Hepp,(1974), one can start by "following" a coherent state along its semiclassical evolution. We shall establish the following result :
starting from a coherent state $|z\rangle$ at time t=0, its quantum evolution stays close to a "squeezed state"

$$\hat{T}(z_t)\hat{R}(F_t)|0\rangle$$

centered around the point $z_t := \phi_H^t(z)$, with a "dispersion" governed by a symplectic matrix F_t that we shall make precise later. This approximation is of order $O(\hbar^\epsilon)$ as long as time doesn't go beyond the so-called **Ehrenfest time** $T_E := \lambda^{-1}\log\hbar^{-1}$. Intuitively the phase-space directions where the wavepacket **spreads** are the unstable directions of the classical flow, whereas those along which they **are squeezed** are the stable ones ; those **stable** and **unstable** directions are encoded in the symplectic matrix F_t.

All that follows will be true for a very general class of Hamiltonians (possibly time-dependent) :

$$\exists m, M, K > 0 : \quad (1+z^2)^{-M/2}|\partial_z^\gamma H(z,t)| \leq K \quad \forall|\gamma| \geq m \tag{3.20}$$

unifomly for $(z,t) \in [-T,T] \times Z$

such that the classical and quantum evolutions respectively (for the classical symbol and its Weyl quantization resp.) exist for $t \in [-T,T]$.

It is well-known that the stability of the classical Hamiltonian evolution governed by H(z, t) is given by the following linear system :

$$\dot{F} = JM_tF \tag{3.21}$$

where M_t is the $2n \times 2n$ Hessian matrix of H at point z_t of the classical trajectory :

$$(M_t)_{j,k} := \left(\frac{\partial^2 H}{\partial z_j \partial z_k}\right)_{j,k}(z_t,t) \tag{3.22}$$

is symmetric real, and the initial datum is

$$F(0) \equiv \mathbb{1} \tag{3.23}$$

Consider the purely quadratic Hamiltonian (time-dependent) :

$$\hat{H}_0(t) := \frac{1}{2}\hat{Z}.M_t\hat{Z} \tag{3.24}$$

It induces a quantum evolution $U_0(t,t')$ via

$$i\hbar\frac{\partial}{\partial t}U_0(t,t') = \hat{H}_0(t)U_0(t,t') \tag{3.25}$$

which is entirely explicit :

Lemma 3.3.1 *Let F_t be the $2n \times 2n$ symplectic matrix solution or equ. (3.21)-(3.23). We note by $\hat{R}(F_t)$ the metaplectic associated operator, unitary in $\mathcal{H}$. We have :*

$$U_0(t,0) = \hat{R}(F_t) \tag{3.26}$$

and therefore by the chain rule :

$$U_0(t,t') = \hat{R}(F_t)\hat{R}(F_{t'}^{-1}) \tag{3.27}$$

This result can be easily obtained by use of the "generalized coherent states" of Perelomov. It encompasses the physical intuition that , for Hamiltonians purely **quadratic** the quantum dynamics is exactly solvable in terms of the classical one. Namely the linear equ. (3.21) is nothing but the classical Hamilton's equations for the quadratic Hamiltonian (3.24).

In fact $\hat{R}(F_t)$ decomposes itself into the product of two unitaries,(built from the symplectic matrix F_t)
-one expressing the "squeezing"
-one expressing the "rotation"

Lemma 3.3.2 *From F_t can be built two $2n \times 2n$ matrices E_t and Γ_t such that :*

$$\hat{R}(F_t) = \hat{S}(E_t)\hat{\mathcal{R}}(t) \tag{3.28}$$

$$\hat{S}(E_t) := \exp\left(\frac{1}{2}(a^\dagger.E_t a^\dagger - a.E_t^* a)\right) \tag{3.29}$$

$$\hat{\mathcal{R}}(t) = \exp\left(\frac{i}{2}(a^\dagger.\tilde{\Gamma} a + a.\Gamma a^\dagger)\right) \tag{3.30}$$

Morally, in dimension n=1, $\hat{\mathcal{R}}(t)$ has the simple form

$$\exp\left(\frac{i\gamma_t}{2}(\hat{Q}^2 + \hat{P}^2)\right)$$

which is simply a rotation by the real angle γ_t.

Let us consider the Taylor expansion up to order 2 of Hamiltonian H(z, t) around the point $z = z_t := (q_t, p_t)$ of the classical trajectory at time t :

$$H_2(t) := H(z_t,t) + (z - z_t).\nabla H(z_t,t) + \frac{1}{2}(z - z_t).M_t(z - z_t) \tag{3.31}$$

By quantization it yields :

$$\hat{H}_2(t) = H(z_t,t)\mathbb{1} + (\hat{Z} - z_t).\nabla H(z_t,t) + \frac{1}{2}(\hat{Z} - z_t).M_t(\hat{Z} - z_t) \qquad (3.32)$$

Let $U_2(t,s)$ be the quantum propagator for Hamiltonian $\hat{H}_2(t)$. We have :

Proposition 3.3.3

$$U_2(t,s) = e^{i(\delta_t - \delta_s)/\hbar}\hat{T}(z_t)\hat{R}(F_t)\hat{R}(F_s^{-1})\hat{T}(-z_s) \qquad (3.33)$$

where

$$\delta_t := S_t(z) - \frac{q_t.p_t - q.p}{2} \qquad (3.34)$$

and $S_t(z) = \int ds(\dot{q}_s.p_s - H(z_s,s))$ *is the classical action along the trajectory* $z \longrightarrow z_t$

In fact this propagator which, being constucted via generators of the coherent/squeezed states acts in a simple manner on coherent states, and appears to be a good approximation of the full propagator $U_H(t,s)$ in the classical limit, when acting on coherent states :

$$\begin{aligned} U_2(t,0) &= e^{i\delta_t/\hbar}\hat{T}(z_t)\hat{S}(E_t)\hat{\mathcal{R}}(t)\hat{T}(-z) \\ U_2(t,0)|z\rangle &= e^{i\delta_t/\hbar}\hat{T}(z_t)\hat{S}(E_t)\hat{\mathcal{R}}(t)|0\rangle \\ &= e^{i\delta_t/\hbar + \gamma_t}\hat{T}(z_t)\hat{S}(E_t)|0\rangle \end{aligned}$$

where $\gamma_t = \frac{1}{2}tr\Gamma_t$
The state

$$\Phi(z,t) := \hat{T}(z_t)\hat{S}(E_t)|0\rangle \qquad (3.35)$$

is simply a squeezed state centered in z_t, with a “squeezing” given by matrix E_t.

Theorem 3.3.4 *Let H be an Hamiltonian satisfying the assumptions (3.20) and the existence of classical and quantum flows for $t \in [-T,T]$. Then we have, uniformly for $(t,z) \in [-T,T] \times Z$:*

$$\|U_H(t,0)\varphi_z - e^{i\delta_t/\hbar + \gamma_t}\Phi(z,t)\| \leq C\mu(z,t)^P|t|\sqrt{\hbar}\theta(z,t)^3 \qquad (3.36)$$

P being a constant only depending on M and m, and

$$\mu(z,t) := Sup_{0\le s\le t}(1+|z_s|)$$

$$\theta(z,t) := Sup_{0\le s\le t}(trF_s^*F_s)^{1/2}$$

The estimate (3.36) contains the dependance in $t, \hbar, z$ of the semiclassical error term. One hopes that this error remains small when $\hbar \to 0$, provided that z belongs to some compact set of phase-space, and $|t|$ is not too large.

Typically

$$\theta(z,t) \simeq e^{t\lambda}$$

where λ is some Lyapunov exponent that expresses the "classical instability" near the classical trajectory. The RHS of equ. (3.36) is therefore $O(\hbar^{\epsilon/2})$ provided

$$|t| < \frac{1-\epsilon}{6\lambda}\log \hbar^{-1} \tag{3.37}$$

which is typically the Ehrenfest time, up to a factor 1/6 that is probably inessential.

Remark 3.3.5 *Theorem (3.3.4) can be modified (and therefore also the state $\Phi(z,t)$) to have an estimate in*

$$\mu(z,t)^{lP}\sum_{j=1}^{l}\left(\frac{|t|}{\hbar}\right)^j(\sqrt{\hbar}\theta(z,t))^{2j+l}$$

and therefore typically $O(\hbar^{l/2})$ with $l \in \mathbb{N}$ as large as one wants. The squeezed state however now depends on l, and is typically a finite linear combination of wavepackets of the form :

$$\hat{T}(z_t)\hat{R}(F_t)|\Psi_\mu\rangle$$

where the Ψ_μ are excited levels of the Harmonic Oscillator in dimension n.

Chapitre 4

A Semiclassical Approach of the so-called Quantum Chaos Problems

4.1 A first view on the problems for Billiards

Billiars are generally planar domains $\Omega \subset \mathbb{R}^2$ with a boundary $\partial\Omega$ piecewise regular. Two kinds of problems, a priori not related, are the following :

•(1) The classical mechanics of a material point moving with constant velocity inside the billiard, with specular reflexions on the boundary

•(2) The wave mechanics inside the billiard, which is related to the Helmhotz problem, namely to the spectral properties of the Laplacean

$$\Delta_\Omega := \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial y_2^2}$$

with Dirichlet boundary conditions on $\partial\Omega$.
This second problem imitates a "quantum problem" with Hamitonian $-\Delta + V$ where the potential V is zero inside Ω and infinite outside of it.

(1) The classical flow of a material point in Ω can be very complicated, and even "unpredictable", as we'll see, in a vast majority of cases.

(2) It is well known since a long time that there exists a basis of orthonormal states of Δ_Ω :

$$-\Delta_\Omega \varphi_j = \lambda_j \varphi_j \qquad \varphi_j \equiv 0 \quad y \in \partial\Omega$$

$$\varphi_j \in L^2(\Omega) \qquad \lambda_0 \leq \lambda_1 \leq ... \leq \lambda_n...$$

with $\lim_{j\to\infty} \lambda_j = \infty$ and that each eigenstate is of finite multiplicity. This collection of $(\lambda_j)_{j\in\mathbb{N}}$ constitutes the discrete spectrum of $-\Delta_\Omega$. The λ_j 's are considered physically as the "energy levels" of the corresponding quantum problem.

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Reed-Simon : vol 4

A natural Question to ask (which is a variant of the famous one addressed by V. Kac : **can we hear the shape of a drum ?**) is the following :

Can one obtain informations, at least statistical ones, on the asymptotic behavior $j \to \infty$ of the λ_j's and φ_j's (Problem (2)) in terms of informations on the classical flow (Problem (1)) ?

Conjecture, (vague) :

• If the classical flow is regular (= predictible), then the spectrum (λ_j) is asymptotically irregular (random, decollerated)

• If the classical flow is irregular (= unpredictible, "chaotic"), then the spectrum (λ_j) is regular (= correlated)

Many numerical experiments corroborate this conjecture. However very few exact results.

A rather general assumption on the classical flow, - the **ergodicity** property that we shall make explicit in the next section - reflects itself in a property of **equidistribution** of the eigenstates φ_j. This result, known as the **Schnirelman Theorem** that we'll expose in Section 3 goes far beyond the case of "billiards", but we shall express it here for the case of billiards, in order to provide a "physical" motivation to this Chapter.

The assumption for the classical flow of being "ergodic" implies that if $B \subset \Omega$ is a measurable subset of Ω, then the mean-time spent by a "typical" trajectory $y \to y_t$ is proportional to the Lebesgue measure $|B|$ of B :

$$\lim_{T\to\infty} T^{-1} |\{t \leq T \ : \ y_t \in B\}| = \frac{|B|}{|\Omega|} \tag{4.1}$$

Under this property, then, "almost surely" the eigenstates φ_j **equidistribute** on Ω asymtotically as $j \to \infty$:

more precisely there exists a subsequence of density 1 of eigenstates φ_{j_k} such that $\forall B \subset \Omega$, measurable, we have :

$$\lim_{k\to\infty} \int_B dy|\varphi_{j_k}(y)|^2 = \frac{|B|}{|\Omega|} \tag{4.2}$$

A strictly monotone sequence of intejers $j_k \in \mathbb{N}$ is said to be "of density one" (or more generally $a < 1$) if

$$\lim_{J\to\infty} J^{-1}\sharp\{k \in \mathbb{N} \ : \ j_k \leq J\} = a$$

Remembering that $\int_\Omega |\varphi_j(y)|^2 dy = 1$, and thus that $|\varphi_j|^2$ represents the quantum probability density at point $y \in \Omega$ we see that morally :

$$\lim_{k\to\infty} |\varphi_{j_k}(y)|^2 = \frac{1}{|\Omega|} \qquad \forall y \in \Omega$$

which expresses the (almost sure) equidistribution of eigenstates φ_j for ergodic billiards, asymptotically when j becomes large.

But which are the ergodic Billiards ?
Clearly circular billiards are **non-ergodic** as can be checked on the figure. So are "elliptic" ones.
On the contrary the "Bunimovitch Billiard , or Stadium (two Half-Circles separated by a strip as small as we want) can be shown to be **ergodic**.
Joyce : J. Acoustic Soc. Am. **58**, 643-655 (1975)
gives a fascinating application of the study of ergodic billiards (in dimension 3) to the Acoustics of an Auditorium !

Une autre façon de penser à la **différence** entre les dynamiques régulière et "chaotique" des 2 billards est la suivante :

• supposons que l'on connaisse la position initiale et la vitesse initiale de la boule de billard seulement avec une précision $\boldsymbol{\varepsilon}$.
Dans le billard **circulaire**, deux données initiales distantes de $\boldsymbol{\varepsilon}$ se séparent **LINÉAIREMENT** au cours du temps ; donc les trajectoires correspondantes seront à une distance de l'ordre de 1 après un temps de l'ordre de $\boldsymbol{\frac{1}{\varepsilon}}$
.
Ceci implique qu'au bout de ce temps, vous avez perdu toute information utile sur votre boule : tout ce que vous pouvez dire c'est qu'elle est **quelque part sur le billard !**
Si $\boldsymbol{\varepsilon = 10^{-4}}$ (ce qui est une très bonne précision pour un joueur de billard !), le temps au bout duquel vous ne pouvez plus prédire où est la boule est de $\boldsymbol{10^4}$ rebonds !

• Pour le billard de Sinai, le temps au bout duquel on a **"perdu le boule"** est de l'ordre de $\boldsymbol{\mathrm{Log}\,\varepsilon}$ ce qui est très peu : **8** rebonds seulement si $\boldsymbol{\varepsilon = 10^{-4}}$. La perte d'information est très rapide dans ce cas.

Une instabilité **exponentielle** comme celle du billard de Sinai se manifeste dans de nombreux systèmes dynamiques et se définit mathématiquement par la notion **d'hyperbolicité**. Elle est souvent appelée **CHAOS DÉTERMINISTE** par la communauté des physiciens. Une telle dynamique est souvent dite aussi **irrégulière**, **imprédictible** ou simplement **chaotique**.

Bibliographie : Tabachnikov , **Billiards** Panorama et Synthèses 1, SMF (1995)

4.2 UN PARFUM DE THÉORIE ERGODIQUE

Les propriétés statistiques de systèmes dynamiques (en termes de leurs mesures invariantes), et tout particulièrement le **comportement à grand temps** des "moyennes" dans l'espace de phase est l'objet de la THÉORIE ERGODIQUE, ce qui est un sujet :

●mathématiquement très bien fondé

●physiquement très fructueux, tant sur le plan des modèles expérimentaux que numériques.

Ce que les physiciens appellent CHAOS, et dont on a vu une illustration avec le billard de Sinai, semble décourager **investigation à grand temps** de la dynamique, du moins si on cherche à suivre des orbites particulières. Néanmoins les propriétés STATISTIQUES permettent de connaître que des points **typiques** de l'espace de phase vont passer un certain temps dans une **région** de l'espace de phase. C'est le B.A.-BA de la **THÉORIE ERGODIQUE**.

En poussant un cran plus loin, on va essayer de voir comment un système "CHAOTIQUE" va, dans un sens **statistique**, faire qu'une dynamique parfaitement DÉTERMINISTE approche en un certain sens, À GRAND TEMPS, un système aléatoire, c'est à dire à quel taux la **MÉMOIRE des conditions initiales** se PERD quand le temps évolue.
C'est le B.A.-BA de la notion de **MÉLANGE** que l'on abordera dans un 2ème temps

Bibliographie :

Cornfeld, Fomin, Sinai. :**Erdodic theory**
Petersen : idem

Walters :**An introduction to ergodic theory**

Dans ce cours on se contentera d'*effleurer* le sujet, afin d'en dégager le PARFUM SUBTIL...

Soit $\boldsymbol{M}$ un espace sur lequel vit une dynamique notée $\boldsymbol{\Phi^t}$:

$$\boldsymbol{a \in M \quad \mapsto \Phi^t\, a \in\ M}$$

et une mesure de probabilité $\boldsymbol{\mu}$ $\quad(\boldsymbol{\mu \geq 0,\ \int_A d\mu = 1})$.

Typiquement, pour un système Hamilttonien classique, d'Hamiltonien $\boldsymbol{H}$, et pour un niveau d'énergie $\boldsymbol{E}$ non-critique ($\boldsymbol{\nabla H \neq 0}$ si $\boldsymbol{H = E}$), on prend :

$\boldsymbol{A = \Sigma_E}$ surface d'énergie

$\boldsymbol{\Phi^t_H}$ flot Hamiltonien engendré par $\boldsymbol{H}$

$\boldsymbol{d\nu := d\sigma_E = \frac{d\Sigma_E}{|\nabla H|}}$ mesure de Liouville

que l'on normalise à $\boldsymbol{1}$ pour donner la mesure microcanonique :

$$\boldsymbol{d\mu = \frac{d\sigma_E}{\int_{\Sigma_E} d\sigma_E}} \tag{4.3}$$

4.2.1 ERGODICITÉ

Definition 4.2.1 *Soit* $\boldsymbol{M}$ *un espace de probabilité, un flot* $\boldsymbol{\Phi^t}$ *défini sur* $\boldsymbol{M}$ *et une mesure de probabilité* $\boldsymbol{\mu}$ *invariante par* $\boldsymbol{\Phi^t}$*. On dit que le système dynamique représenté par* $\boldsymbol{(M, \Phi^t, \mu)}$ *est ergodique si pour toute fonction* $\boldsymbol{f}$ *définie sur* $\boldsymbol{M}$*, suffisamment régulière, la moyenne de* $\boldsymbol{f}$ *le long d'une* *orbite quelconque dans* $\boldsymbol{M}$ *est indépendante du point de départ* $\boldsymbol{a}$ *de l'orbite (à* $\boldsymbol{t = 0}$*), pour* $\boldsymbol{\mu}$ *-presque tout* $\boldsymbol{a}$ *et égale la moyenne de* $\boldsymbol{f}$ *sur* $\boldsymbol{M}$ *:*

$$\lim_{T\to\infty} T^{-1} \int_0^T dt\ f(\Phi^t a) = \int_M f(z)\ d\mu(z) \qquad (4.4)$$

pour $\boldsymbol{\mu}$*-presque tout* $\boldsymbol{a \in M}$

Remark En réalite ceci constitue le *Théorème ergodique de Birkhoff.*

On a vu au paragraphe précédent que la dynamique classique sur un billard circulaire ou elliptique est non-ergodique (ces billards sont **classiquement complètement intégrables**), mais que la dynamique sur le billard de Bunimovitch est ergodique. On s'attend à ce qu'elle soit même **très irrégulière**, et une première approche de cette notion d'irrégularité (ou **chaos**) est la propriété de MÉLANGE.

4.2.2 Le MÉLANGE comme une mesure de l'irrégularité de la dynamique

Question (Q) : Soient $\boldsymbol{A}$ et $\boldsymbol{B}$ deux sous-ensembles de $\boldsymbol{M}$ ($\boldsymbol{M}$ par ex. surface d'énergie). Á un instant $\boldsymbol{t}$ donné, quelle est le probabilité pour une trajectoire ayant démarré en un point $\boldsymbol{a}$ de $\boldsymbol{B}$, d'aboutir dans $\boldsymbol{A}$ à l'instant $\boldsymbol{t}$?

$$(a \in B \qquad \Phi^t a \in A)$$

Intuitivement, si la dynamique est **imprédictible à long terme**, alors on ne sait pas prévoir où les trajectoires vont aller plus $\boldsymbol{t}$ est grand, et donc la réponse ne devrait pas dépendre **d'où** $\boldsymbol{A}$ est situé sur $\boldsymbol{M}$.

ni d'ailleurs de la **position**, de la **forme** ou de la **taille** de $\boldsymbol{B}$.

Par contre la réponse à la question (**Q**) dépend de la **taille** de $\boldsymbol{A}$:

(si $\boldsymbol{A} = \boldsymbol{M}$ alors cette probabilité est évidemment égale à $\mathbf{1}$, tandis que si $\boldsymbol{A}$ est petit, elle sera nécessairement petite.)

$\boldsymbol{\mu}$ étant une mesure de probabilité, la quantité :

$$\frac{\boldsymbol{\mu(\Phi^t(B) \cap A)}}{\boldsymbol{\mu(B)}} \tag{4.5}$$

est donc la fraction de toutes les trajectoires partant de $\boldsymbol{B}$ (à l'instant $\mathbf{0}$) et aboutissent dans $\boldsymbol{A}$ à l'instant $\boldsymbol{t}$.

On s'attend donc, pour une dynamique **imprédictible à long terme**, à ce que cette fraction (2) égale la TAILLE de $\boldsymbol{A}$ (au sens de la mesure $\boldsymbol{\mu}$, ie $\boldsymbol{\mu(A)}$). D'où la propriété :

$$\lim_{t\to\infty} \frac{\boldsymbol{\mu(\Phi^t(B) \cap A)}}{\boldsymbol{\mu(B)}} = \boldsymbol{\mu(A)} \tag{4.6}$$

CETTE PROPRIÉTÉ EST APPELÉE PROPRIÉTÉ DE MÉLANGE

(au sens fort ; il existe des versions “faibles” de cette propriété).

Definition 4.2.2 *Le flot Hamiltonien $\boldsymbol{\Phi_H^t}$ est dit MÉLANGEANT sur la couche d'énergie $\boldsymbol{\Sigma_E}$ si quels que soient $\boldsymbol{A},\ \boldsymbol{B} \subset \boldsymbol{\Sigma_E}$ mesurables, on a :*

$$\lim_{t\to\infty} \boldsymbol{\mu_E(\Phi_H^t \cap A) = \mu_E(B)\mu_E(A)} \tag{4.7}$$

où $\boldsymbol{\mu_E}$ est la mesure microcanonique sur $\boldsymbol{\Sigma_E}$ définie par (1).

Remarque : Cette notion reste encore assez vague, bien que fortement intuitive (voir figure). En effet, la dynamique sera d'autant plus **imprédictible à long terme** que la limite (5) sera atteinte rapidement. Le summum étant le MÉLANGE EXPONENTIEL, où :

$$\mu_E(\Phi_E^t(B) \cap A) - \mu_E(A)\mu_E(B) \sim Ce^{-\gamma t} \tag{4.8}$$

pour un C et $\gamma > 0$

4.2.3 INSTABILITÉ EXPONENTIELLE $\Rightarrow^?$ MÉLANGE EXPONENTIEL

On s'attendrait à ce qu'une INSTABILITÉ EXPONENTIELLE de la dynamique, au sens de l'existence d'exposants de Lyapunov positifs, implique le MÉLANGE EXPONENTIEL.

It is well-known that if a system has vanishing Lyapunov exponents, then the DECAY of correlations can be arbitrarily slow. (Collet-Eckmann, 2003)

Ce problème est en réalité beaucoup plus subtil que cela n'en a l'air, et nous n'entrerons pas plus avant dans le sujet.

Definition 4.2.3 *(autre formulation de la PROPRIÉTÉ DE MÉLANGE)*

$$\forall f,\ g \in L^2(\Sigma_E,\ d\mu_E)$$

we have :

$$\lim_{t\to\infty}\left(\int_{\Sigma_E} d\mu_E(z)\ f\circ\Phi_H^t(z)\ g(z) - \int_{\Sigma_E} d\mu_E(z)\ f(z)\ \int_{\Sigma_E} d\mu_E(z)\ g(z)\right) \tag{4.9}$$

La quantité entre parentheses de (4.9) s'appelle la **fonction de corrélation classique** *de f et g à l'instant t (ou fonction d'autocorrélation si $f = g$).*

Lemma 4.2.4 *Si le flot Hamiltonien Φ_H^t est MÉLANGEANT sur Σ_E, alors il est aussi ergodique (pour la mesure microcanonique). Plus généralement :*

$(A,\ \Phi^t,\ \mu)$ *mélangeant* $\Rightarrow$ $(A,\ \Phi^t,\ \mu)$ *ergodique*

Preuve : (cas discret : $\Phi^t = T^n$ pour une “évolution en temps discret” T et $n \in \mathbb{N}$)
Montrons que $(A,\ T,\ \mu)$ est ergodique
$\Longleftrightarrow\ \lim_{n\to\infty} \sum_0^{n-1} \mu(T^{-j}A \cap B) = \mu(A)\mu(B)$.

On a, en prenant pour f la fonction caractéristique de l'ensemble A : χ_A

$$\lim_{n\to\infty} \sum_0^{n-1} \chi_A(T^{-j}x) = \mu(A) \tag{4.10}$$

On multiplie par χ_B, puis on intègre sur x :

$$\frac{1}{n} \sum_0^{n-1} \chi_A(T^{-j}x)\chi_B(x) \to \mu(A)\chi_B(x) \tag{4.11}$$

$$\frac{1}{n} \sum_0^{n-1} (T^{-j}A \cap B) \to \mu(A)\ \mu(B)$$

quand $n \to \infty$.

Or,on a : $a_n \to 0\ \Rightarrow \frac{1}{n}\sum_0^n a_j \to 0$, et le résultat suit en prenant :

$$a_n = \mu(T^{-n}A \cap B) - \mu(A)\mu(B)$$

Exemple Il a été prouvé que le billard de Sinai est mélangeant.

En réalité la propriété de MÉLANGE a été prouvée pour peu de systèmes Hamiltoniens en temps continu. C'est pourquoi beaucoup d'auteurs se sont intéressés à des **systèmes dynamiques en temps discret** qui préservent la mesure de façon à imiter au mieux le flot Hamiltonien ;

par exemple des dynamiques discrètes sur le tore comme :

- le CHAT d'Arnold
- la transformation dite du BOULANGER

De même que l'ERGODICITÉ classique exprime **l'équidistribution** à grand temps des **trajectoires classiques** sur le domaine de l'espace de phase disponible (usuellement la SURFACE D'ÉNERGIE $\boldsymbol{\Sigma_E}$) ,

de même le THÉORÈME DE SCHNIRELMAN en est une traduction "SEMICLASSIQUE" en terme **d'équidistribution** sur $\boldsymbol{\Sigma_E}$ des **fonctions propres du Hamiltonien quantique**.

4.3 Le Théorème de Schnirelman

Esquissé plus haut dans le cas particulier des billards, le théorème de Schnirelman exprime que :

L'**Ergodicité** du flot $\Rightarrow$ L'**Équidistribution** des fonctions propres

CLASSIQUE du HAMILTONIEN QUANTIQUE

A LA LIMITE $\boldsymbol{\hbar \to 0}$

(dans le cas des billards, la LIMITE SEMICLASSIQUE était simplement l'asymptotique à Haute Énergie)

Depuis sa formulation par Schnirelman en **1974**, le théorème a connu beaucoup d'AVATARS (au sens étymologique de “réincarnations successives” !), en particulier dans :

• l'Opérateur de Laplace-Beltrami sur des variétés compactes à courbure négative

• des Billards à courbure irrégulière

• des Opérateurs de Schrödinger à potentiel régulier

Assumptions

(H1) $H(\hbar, z) \asymp \sum_{j=0}^{\infty} \hbar^j H_j(z) \qquad H_j : Z \mapsto \mathbb{R} \in \mathcal{C}^\infty(Z)$

(H2) H_0 bounded from below and

$0 \leq H_0(z) + \gamma_0 \leq C(H_0(z') + \gamma_0)(1 + |z - z'|)^M \quad \forall z, z' \in Z$

(H3) $\forall j \in \mathbb{N},\ \forall \gamma \in \mathbb{N}^{2n} \quad |\partial_z^\gamma H_j(z)| \leq C(H_0(z) + \gamma_0)$

(H4) $|\partial_z^\gamma (H(\hbar, z) - \sum_0^N \hbar^j H_j(z))| \leq C(N, \gamma)\hbar^{N+1} \quad \forall \hbar \in (0, 1)$ uniformly for $z \in Z$

(H5) Let $I_{cl} :=]\lambda_-, \lambda_+[$ be an interval of classical energy, then $H_0^{-1}(I_{cl})$ is bounded in $\mathbb{R}^{2n}$ (the energy surfaces for $E \in I_{cl}$ are all compact)

(H6) E is a noncritical value for H_0 namely $H_0(z) = E \Rightarrow \nabla_z H_0 \neq 0$

(H7) The dynamical system $(\Sigma_E, dLE, \phi^t_{H_0})$ is ergodic (recall that dLE is the Liouville measure defined in (1.4))

Let $\hat{H}$ be the Weyl quantization of $H(\hbar, z)$. It is a selfadjoint operator in $\mathcal{H}$. The assumptions H1-H5 imply that for any interval $J \subset I_{cl}$ and for $\hbar$ small enough, the spectrum of $\hat{H}$ in J is pure point :

$$sp(\hat{H}) \bigcap J = \{E_j(\hbar)\}_{j=1}^N \qquad for N := N(\hbar) = O(\hbar^{-n})$$

Denote by φ_j the corresponding eigenstates.

Lemma 4.3.1 *Let* $J = [E_-, E_+]$ *with* $E_\pm$ *non critical for* H_0*. We have :*

$$N_J(\hbar) = h^{-n} Vol_Z(H_0^{-1}(J)) + O(\hbar^{1-n}) \tag{4.12}$$

Which is known as the **Weyl asymptotic formula**

Intuition A quantum state in $\mathcal{H}$ occupates a phase-space volume of size h^n, as we have for instance explicited for coherent states. Thus a volume $A \subset Z$ contains $\frac{Vol(A)}{h^n}$ "quantum states" asymptotically as $h \longrightarrow 0$.

We shall now consider a small energy interval around $E \in I_{cl}$:

$$I(\hbar) = [E - \delta(\hbar), E + \delta(\hbar)] \tag{4.13}$$

where $\delta(\hbar) \geq \epsilon\hbar$ for some $\epsilon > 0$.

$$\Lambda(\hbar) := \{j \ : \ E_j(\hbar) \in I(\hbar)\} \tag{4.14}$$

$$N_\hbar = \sharp\Lambda(\hbar) \tag{4.15}$$

Consider $A \in \mathcal{O}(0)$ a classical observable, with $\hat{A}$ its Weyl quantization. We define :

$$A_{j,k} := \langle \varphi_j, \hat{A}\varphi_k \rangle \tag{4.16}$$

the matrix element of $\hat{A}$ in the eigenstates of $\hat{H}$ for $j, k \in \Lambda(\hbar)$

Theorem 4.3.2 Schnirelman Theorem
Under assumptions H1-H7 for H, and for any classical observable $A \in \mathcal{O}(0)$, $\forall\hbar$ *sufficiently small* $\exists M(\hbar) \subseteq \Lambda(\hbar)$ *depending only on H such that :*

$$\lim_{\hbar\to 0} \frac{\sharp M(\hbar)}{\sharp\Lambda(\hbar)} = 1 \tag{4.17}$$

and

$$\lim_{\hbar\to 0} A_{j,j} = \int_{\Sigma_E} A(z)\, dL_E(z) \tag{4.18}$$

We shall not give here the proof that is relatively sophisticated. We shall content ourselves to indicate in which respect this expresses the "almost sure" equidistribution of eigenstates φ_j on Σ_E.

We have shown that, by denoting W_{φ_j} the Wigner distribution associated to some eigenstate $\varphi_j \in \mathcal{H}$:

$$\langle \varphi_j, \hat{A}\varphi_j \rangle = \int_Z A(z) W_{\varphi_j}(z) dz \tag{4.19}$$

Therefore rewritting the RHS of (4.18) as

$$\frac{\int_Z A(z)\delta(H(z) - E)dz}{\int_Z \delta(H(z) - E)dz}$$

we see that, at least along the subsequence of j's in $M_j(\hbar)$:

$$\lim_{\hbar \to 0, j \to \infty} W_{\varphi_j}(z) = \frac{1}{|\Sigma_E|}\delta(H(z) - E) \tag{4.20}$$

which "morally" expresses the almost sure **equidistribution** semiclassically in phase space in the highly excited levels φ_j on the energy shell Σ_E.

We can say a bit more when the system is not only **ergodic** but also **mixing** :

Theorem 4.3.3 *Under assumptions H1-H6, and that the classical flow is* **mixing** *on Σ_E, (property (3.42)), then $\forall A \in \mathcal{O}(m)$, we have for $M(\hbar)$ as in Theorem 4.3.2 that $\forall j \in M(\hbar),\ k \in \Lambda(\hbar),\ j \neq k$:*

$$\lim_{\hbar \to 0, j,k \to \infty} A_{j,k} = 0 \tag{4.21}$$

This expresses that the off-diagonal terms of any observable $\hat{A}$ vanish at the semiclassical limit, even for unbounded observables.

Chapitre 5

Trace Formulas. Mathematical Approach

5.1 First Prototype : The Poisson summation Formula

Under suitable definition of the Fourier Transform $f \longrightarrow \tilde{f}$, we have :

$$\sum_{n=-\infty}^{+\infty} f(n) = \sum_{k=-\infty}^{+\infty} \tilde{f}(2k\pi) \tag{5.1}$$

which holds true for any $f \in \mathcal{S}(\mathbb{R}^n)$ (that implies of course that also $\tilde{f} \in \mathcal{S}(\mathbb{R}^n)$), and which is therefore perfectly symmetric between $f, \tilde{f}$.

Why do we mean that it is a Trace Formula ?

Consider the quantum operator in dimension 1 : $\hat{P} = -i\frac{d}{dx}$ acting on $L^2([0, 2\pi])$, with periodic boundary conditions $u(0) = u(2\pi)$. It is an unbounded operator, whose spectrum if purely discrete :

$$sp(\hat{P}) = \mathbb{Z}$$

Therefore the LHS of equ. (4.1) is nothing but $tr f(\hat{P})$.

What does the RHS represents physically ?

Imagine a classical Hamiltonian $H(q,p) := p$, where $q \in [0, 2\pi]$. ($\hat{P}$ is actually the Weyl quantization (for $\hbar = 1$) of H in $L^2([0, 2\pi])$ with Periodic Boundary conditions).

The associated Hamilton's equations are

$$\dot{q} = 1 \ , \ \dot{p} = 0$$

anf thus : $q = t \qquad (mod\ 2\pi)$

The classical trajectories are thus all closed ie periodic in phase space, and are **k-repetitions** of the primitive orbit of period $2\pi, \qquad \forall k \in \mathbb{Z}$. This means that the periods of the classical flow are of the form $2k\pi \quad k \in \mathbb{Z}$.

The summation Poisson Formula thus expresses that the **trace of a function of a quantum Hamiltonian** of a very peculiar form is **the sum on the periodic orbits of the corresponding classical flow** of the Fourier Transform of that function taken at the periods of the classical flow.

5.2 Second Prototype : The Harmonic Oscillator in dimension 1

$$\hat{H}_0 := \frac{\hat{P}^2 + \hat{Q}^2}{2} \tag{5.2}$$

acting in $L^2(\mathbb{R})$ has spectrum $n + \frac{1}{2}$ (here again we let $\hbar = 1$), where $n \in \mathbb{N}$.

Take $f \in \mathcal{S}([0, +\infty])$. Then obviously

$$tr f(\hat{H}_0) = \sum_{n=0}^{\infty} f(n + \frac{1}{2}) \tag{5.3}$$

Replace f by $\hat{T}(q, 0)f = f(. + q)$ in equ. (5.1). It becomes

$$\sum_{n \in \mathbb{Z}} f(n + q) = \sum_{k \in \mathbb{Z}} e^{2i\pi kq} \tilde{f}(2k\pi)$$

Thus taking $q = 1/2 \qquad e^{ik\pi} = (-1)^k$ which yields :

$$\sum_{n=0}^{\infty} f(n + \frac{1}{2}) = \sum_{k \in \mathbb{Z}} (-1)^k \tilde{f}(2k\pi) \tag{5.4}$$

Since the classical trajectories of the classical Harmonic Oscillator are of the form

$$q(t) = Asin(t + \alpha)$$

every orbit is therefore periodic, with a period which is a k-repetition of the primitive orbit of period 2π. The periods of the closed orbits of the classical flow are thus $\{2k\pi\}_{k \in \mathbb{Z}}$.

We see here a factor $(-1)^k \equiv e^{(2k)i\pi/2}$ which is here the first manifestation of a "Maslov Index" $2k$.

Here again, equ. (5.3) expresses that the trace of the function of a Quantum Hamiltonian can be written as a sum over the periodic orbits of the corresponding classical flow of the Fourier Transform of that function, taken at the periods of the classical flow, **up to some factor of the form $e^{\sigma_k i\pi/2}$ where σ_k is the Maslov index of the orbit**.

5.3 Generalisation. The case of classically chaotic Systems

The examples provided in the two previous sections are in dimension 1 and therefore integrable, since the "energy" is the unique conserved quantity, but there can be only one in this case. For systems in dimension $n > 1$ that are completely integrable, ie have exactly **n conserved quantities** (among which is the energy), the space-phase is folliated into n invariant tori determined by the conserved quantities, and Berry-Tabor have heuristically established that the trace of $f(\hat{H})$ (or the so-called "density of states" in the sense of distributions) is written as a sum on the invariant tori of quantities involving $\tilde{f}$ and characteristics of these tori. The mathematical proof of it was in advance, since in 1973, Colin de Verdière established the result for compact manifolds.

In the case of non-completely integrable systems, thus having some "chaotic properties" in the rather vague physical terminology, Poincaré was the first to notice, in the very beginning of the last century, that the family of **periodic orbits**, generally **unstable** constitutes the "skeleton" around which the dynamics organizes so to say, although it is in general rather irregular and unpredictable.

However this remark has remained largely ignored until the years 1972-73, where independently, Balian and Bloch, and Gutzwiller proposed **Trace Formulae** for these systems, as a (highly divergent) sum over the unstable periodic orbits of the classical flow (and thus on the "skeleton"of the corresponding classical dynamics), of quantities involving :

-The periods of these orbits

-The classical action along these orbits

- Maslov indices for them

-The so-called "Poincaré map" or monodromy matrix of these orbits.

Rigorous proofs of such Trace Formulas were multiple, and do not overcome the difficulties inherent to the exponential proliferation of such orbits when time (period) becomes large. Contrarily to the formulas (5.1) and (5.3) they violate the **symmetry** between $\boldsymbol{f}$, $\tilde{\boldsymbol{f}}$, and thus the quantum/classical symmetry. In the Semiclassical Trace Formulae, $\tilde{\boldsymbol{f}}$ is assumed to have compact support, which has the effect of truncating the sum on periodic orbits, since $\tilde{\boldsymbol{f}}(\boldsymbol{T_\gamma}) = \mathbf{0}$ for $\boldsymbol{T_\gamma}$, the period of the closed orbit $\boldsymbol{\gamma}$, being sufficiently large.

Let us open for a while a heuristic parenthesis on billiards

For billiards, the "quantum/classical duality" of trace formulae is expressed in terms of

-The wave-number $\boldsymbol{k}$ for the quantum equation $(-\boldsymbol{\Delta_\Omega} + \boldsymbol{k^2})\boldsymbol{\psi} = \mathbf{0}$

-The lengths $\boldsymbol{L_j}$ of the periodic orbits inside $\boldsymbol{\Omega}$.

On the quantum side :
In the sense of distributions, the "density of states" (or rather the density of wavenumbers) is :

$$\rho(k) := \sum_n \delta(k - k_n)$$

where the k_n's satisfy

$$(-\Delta_\Omega + k_n^2)\psi_n = 0, \qquad \psi_n \in L^2(\Omega)$$

The dominant (semiclassical) term of $\rho(k)$ is the Weyl term of the form

$$\bar{\rho}(k) = C_d|\Omega|k^{d-1}, \qquad \Omega \in \mathbb{R}^d$$

ie for billiards in dimension d.

We are interested in the fluctuations, or oscillations of $\rho(k)$ around its semiclassical mean value $\bar{\rho}(k)$:

$$\rho^{osc}(k) := \rho(k) - \bar{\rho}(k)$$

On the classical side :

The "classical spectrum" of lengths of periodic orbits indide Ω is denoted $\{L_j\}$.(note that there is a priori no operator of which it is the "spectrum" in the spectral theory of operators sense, and thus it is an abuse of language, just put forward in order to manifest the **duality quantum/classical**). To each L_j corresponds a primitive orbit of length L_p :

$$L_j = rL_p, \quad r \in \mathbb{N}^*$$

and we denote $\nu_j,\ M_j$ the Maslov index and Monodromy matrix respectively. We assume ("Gutzwiller Hypothesis") that M_j doesn't have eigenvalue 1. Let A_j be of the following form :

$$A_j := \frac{L_p e^{i\nu_j\pi/2}}{|\det(M_j - \mathbb{1})|^{1/2}} \tag{5.5}$$

One defines a classical distribution of length with the help of these weigths A_j :

$$\rho_{cl}(L) := \sum_j A_j \delta(L - L_j)$$

and as in the quantum case we substract to it its "mean value" in a suitable sense, thus defining :

$$\rho_{cl}^{osc}(L) = \rho_{cl}(L) - \bar{\rho}_{cl}(L)$$

Then the **quantum/classical duality** is expressed via a Semiclassical Trace Formula which is simply, in distributional sense :

$$\rho^{osc}(k) \sim_{k\to\infty} \mathcal{F}\rho_{cl}^{osc}(L) \tag{5.6}$$

where by $\mathcal{F}$ we simply denote the Fourier Transform.

We close this parenthesis on this formula which seems rather appealing, although completely heuristic, and gives the flavor of what a Semiclassical Trace Formula can be.

In what follows we give a mathematical content to Semiclassical Trace Formula, in the case of regular Hamiltonian Systems.

Theorem 5.3.1 *Let H satisfy (H1)-H6, and $\hat{H}$ its Weyl quantization. Consider the classical flow $\phi_{H_0}^t$ of H_0 on $\Sigma_E : \{H_0(z) = E\}$, and denote by γ the periodic orbits of this flow. We assume in addition (Gutzwiller Hypothesis) that the Poincaré map P_γ doesn't have 1 as eigenvalue, namely that the orbits γ are* **nondegenerate**. *Then for any $\varphi \in \mathcal{S} : \tilde{\varphi} \in \mathcal{C}_0^\infty$, we have, asymptotically as $\hbar \to 0$:*

$$tr\varphi\left(\frac{\hat{H} - E}{\hbar}\right) \asymp h^{-n}\left(\tilde{\varphi}(0)|\Sigma_E|\hbar + \sum_{j\geq 2}\hbar^j c_{0,j}(\tilde{\varphi})\right) \tag{5.7}$$

$$+\sum_\gamma \frac{e^{iS_\gamma/\hbar} + i\sigma_\gamma\pi/2}{|\det(\mathbb{1} - P_\gamma)^{1/2}|}\left(\tilde{\varphi}(T_\gamma)\frac{T_\gamma^*}{2\pi}e^{-i\int_\gamma H_1} + \sum_{j\geq 1}\hbar^j c_{\gamma,j}(\tilde{\varphi})\right)$$

where :
γ^* *is the primitive orbit corresponding to* γ
T_γ *(resp. T_γ^*) is the period of γ (resp. γ^*)*
σ_γ *is the Maslov index of* γ
S_γ *is the classical action along* γ
P_γ *is the Poincaré map of* γ
$c_{0,j}$ *are distributions supported in* $\{0\}$
$c_{\gamma,j}$ *are distributions supported in* $\{T_\gamma\}$

Note that the duality Quantum/Classical is violated by the condition that $\tilde{\varphi}$ is of compact support.
The First line of (5.7) corresponds to the "regular part" in $\hbar$, and we recognize the dominant Weyl term (with corrections in $\hbar$ that Gutzwiller had "omitted", or neglected...)
The Second line corresponds to the "oscillating part" in $\hbar$, which is, as expected, a sum over the periodic orbits of the classical flow (here truncated since $\tilde{\varphi}(T_\gamma) = 0$ for γ large).

The first proofs of Theorem 5.3.1 used the sophisticated theory of FIO, and thus encounters "caustic problems". We shall indicate very briefly how the use of **coherent states** allows to work entirely in phase-space, and thus avoids this difficulty.

$$tr\varphi\left(\frac{\hat{H}-E}{\hbar}\right) = tr\left(\int dte^{it(E-\hat{H})/\hbar}\tilde{\varphi}(t)\right)$$

$$= h^{-n}\int dte^{itE/\hbar}\tilde{\varphi}(t)\int_Z dz\langle z|e^{-it\hat{H}/\hbar}|z\rangle$$

Replacing the expectation value in $|z\rangle$ by its semiclassical approximation, we can replace it (to dominant order in $\hbar$) by :

$$e^{i\gamma_t+i\delta_t/\hbar}\langle z|\Phi(z,t)\rangle$$

The above scalar product is explicit since $\Phi(z,t)$ is simply Gaussian, and therefore the overall integrand in (t,z) is ot the form

$$amplitude \times e^{iPhase/\hbar}$$

and we can use Stationary Phase Theorems. The **Phase** will be stationary iff

$$z = z_t \qquad z \in \Sigma_E$$

which leads to the first line for $t = 0, \quad z \in \Sigma_E$
and to the second line if $t = T_\gamma, \quad z \in \gamma \in \Sigma_E$.